Optimization Techniques for ML

CS771: Introduction to Machine Learning

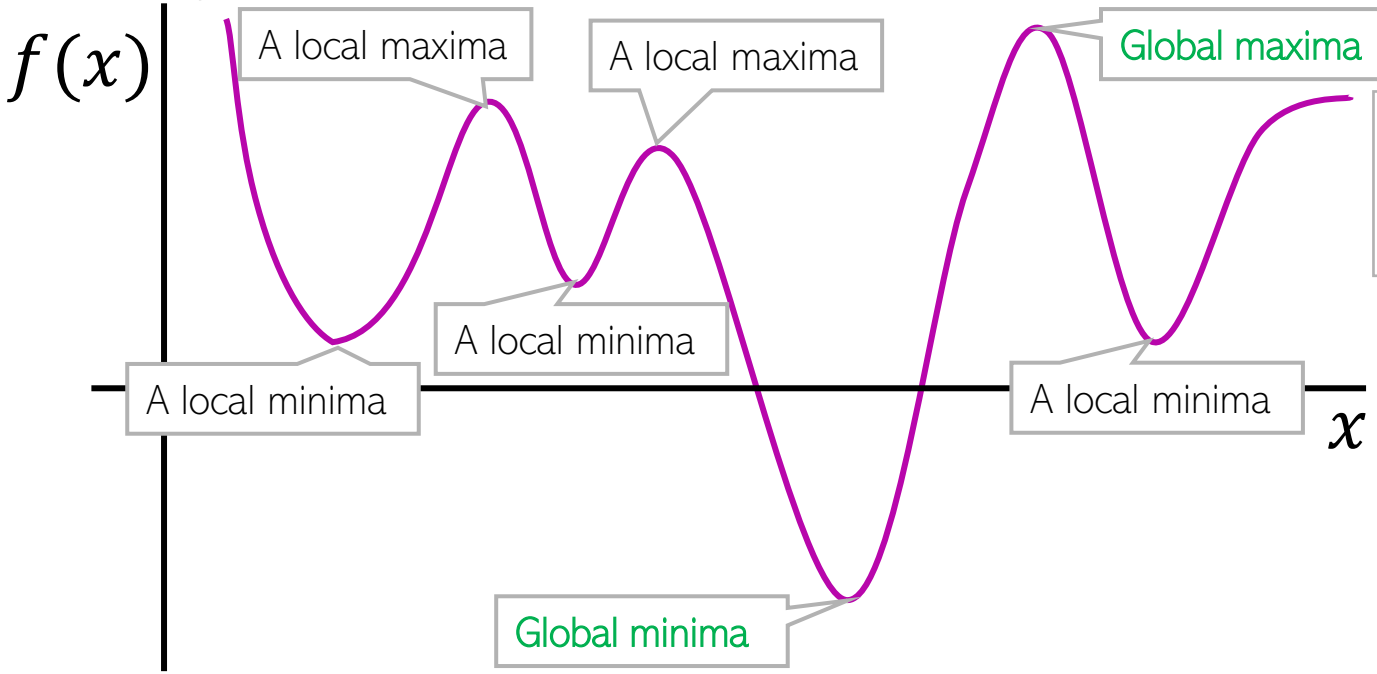
Piyush Rai

Functions and their optima

The objective function of the ML problem we are solving (e.g., squared loss for regression)

Assume unconstrained for now, i.e., just a real-valued number/vector

- Many ML problems require us to optimize a function f of some variable(s) x
- For simplicity, assume f is a scalar-valued function of a scalar x ($f: \mathbb{R} \rightarrow \mathbb{R}$)



Usually interested in global optima but often want to find local optima, too

For deep learning models, often the local optima are what we can find (and they usually suffice) – more later

Will see what these are later

- Any function has one/more optima (maxima, minima), and maybe saddle points
- Finding the optima or saddles requires derivatives/gradients of the function

Derivatives

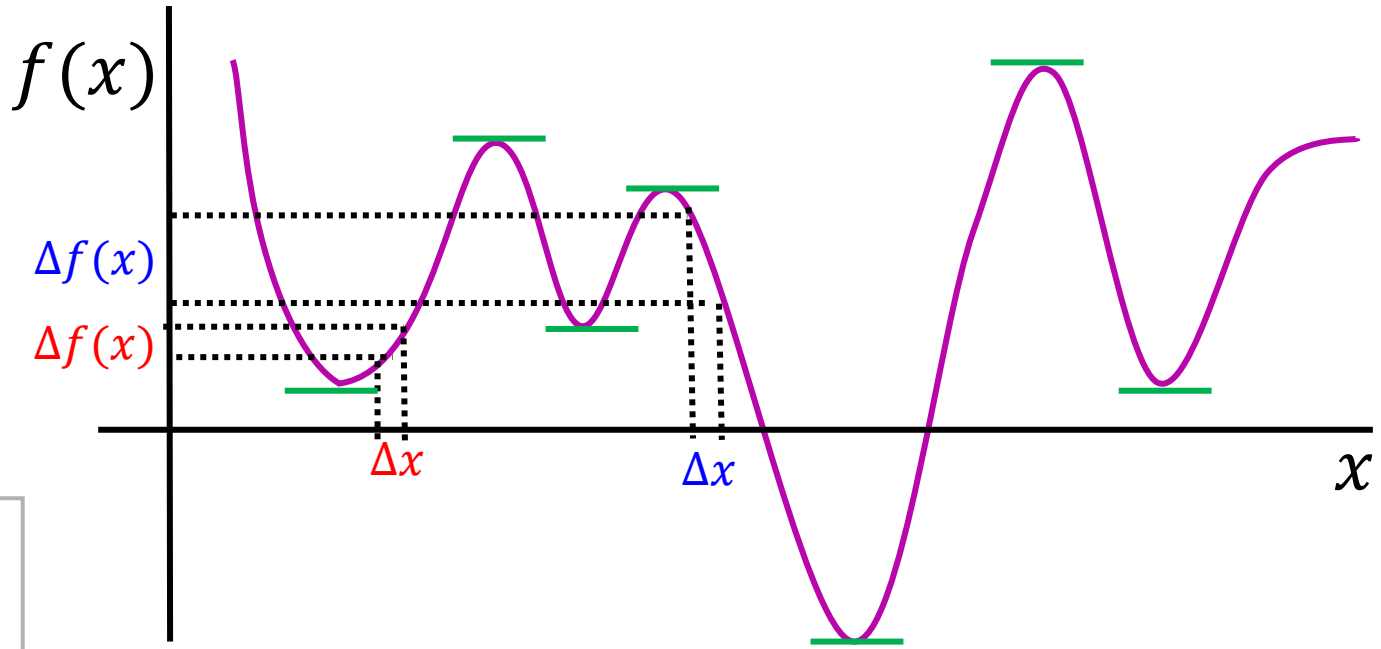
Will sometimes use $f'(x)$ to denote the derivative

- Magnitude of derivative at a point is the rate of change of the func at that point

$$\frac{df(x)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x}$$

Sign is also important: Positive derivative means f is increasing at x if we increase the value of x by a very small amount; negative derivative means it is decreasing

Understanding how f changes its value as we change x is helpful to understand optimization (minimization/maximization) algorithms

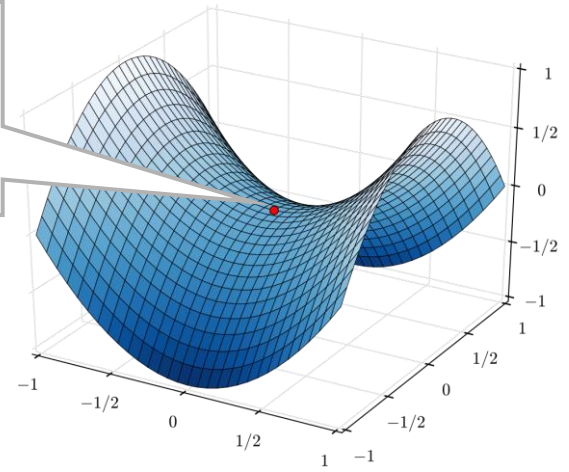


- Derivative becomes zero at stationary points (optima or saddle points)
  - The function becomes "flat" ($\Delta f(x) = 0$ if we change x by a very little at such points)
  - These are the points where the function has its maxima/minima (unless they are saddles)

Saddle Points

- Points where derivative is zero but are neither minima nor maxima

Function might increase along one direction but decrease in a different direction



- Saddle points are very common for loss functions of deep learning models
  - Need to be handled carefully during optimization

- Second or higher derivative may help identify if a stationary point is a saddle

Rules of Derivatives

Some basic rules of taking derivatives

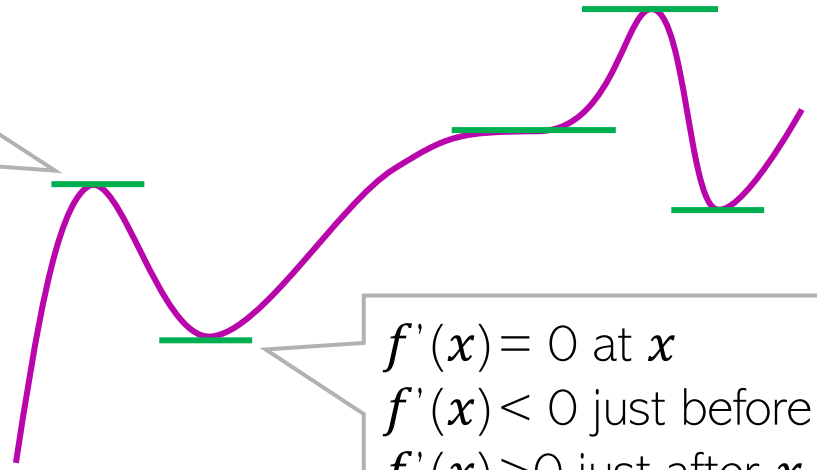
- Sum Rule: $\big(f(x)+g(x)\big)' = f'(x)+g'(x)$
- Scaling Rule: $\big(a \cdot f(x)\big)' = a \cdot f'(x)$ if a is not a function of x
- Product Rule: $\big(f(x) \cdot g(x)\big)' = f'(x) \cdot g(x) + g'(x) \cdot f(x)$
- Quotient Rule: $\big(f(x)/g(x)\big)' = \big(f'(x) \cdot g(x) - g'(x)f(x)\big)/\big(g(x)\big)^2$
- Chain Rule: $\Big(f\big(g(x)\big)\Big)' \stackrel{\text{def}}{=} (f \circ g)'(x) = f'\big(g(x)\big) \cdot g'(x)$

We already used some of these (sum, scaling and chain) when calculating the derivative for the linear regression model

Derivatives

- How the derivative itself changes tells us about the function's optima

$f'(x) = 0$ at x,
$f'(x) > 0$ just before x
$f'(x) < 0$ just after x
x is a maxima



$f'(x) = 0$ at x
$f'(x) < 0$ just before x
$f'(x) > 0$ just after x
x is a minima

$f'(x) = 0$ and $f''(x) < 0$
x is a maxima

$f'(x) = 0$ and $f''(x) > 0$
x is a minima

But, the behavior of second derivative alone may not be enough to tell whether it's a saddle point

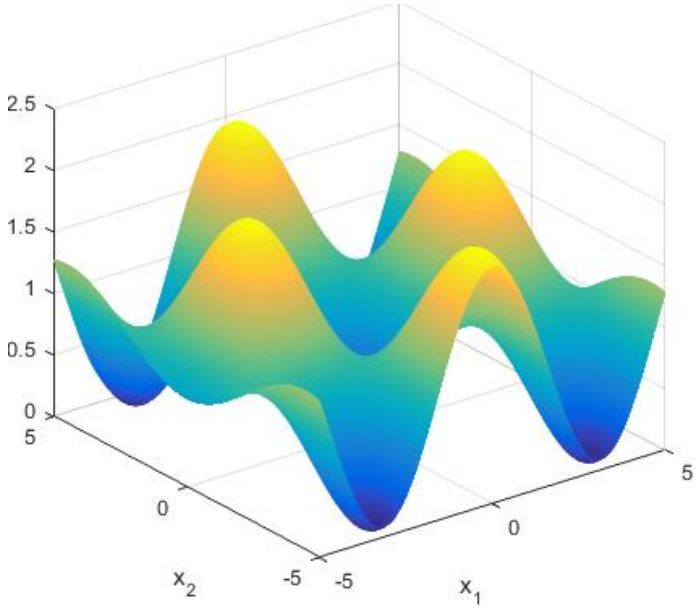
- The second derivative $f''(x)$ can provide this information
  - It is the rate of change of the first derivative

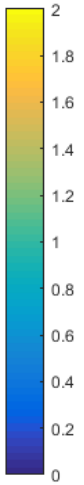
Multivariate Functions

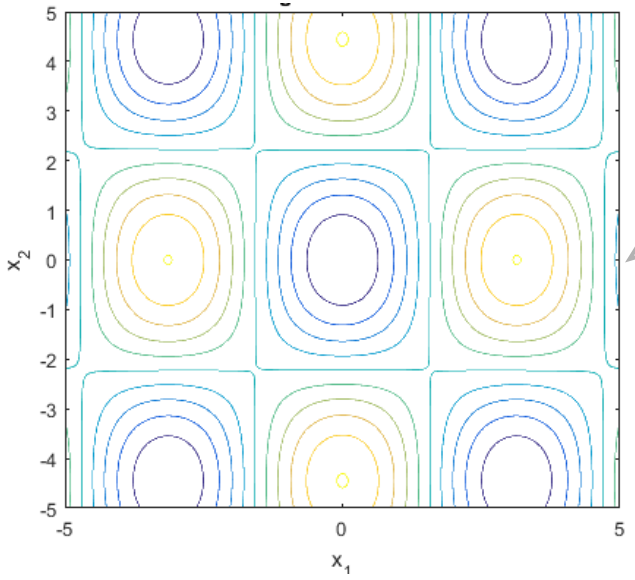
- Most functions that we see in ML are multivariate function
- Example: Loss fn $\boldsymbol{L(w)}$ in lin-reg was a multivar function of $\boldsymbol{D}$-dim vector $\boldsymbol{w}$

$$\boldsymbol{L(w)}: \mathbb{R}^D \rightarrow \mathbb{R}$$

- Here is an illustration of a function of 2 variables (4 maxima and 5 minima)







Two-dim contour plot of the function (i.e., what it looks like from the above)

Each curve here is the set of points at which the function has the same value

Plot courtesy: http://benchmarkfcns.xyz/benchmarkfcns/griewankfcn.html

Derivatives of Multivariate Functions

- Can define derivative for a multivariate functions as well via the gradient
- Gradient of a function $f(\boldsymbol{x})$: $\mathbb{R}^D \rightarrow \mathbb{R}$ is a $D \times 1$ vector of partial derivatives

$$\nabla f(\boldsymbol{x}) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_D}\right)$$

Each element in this gradient vector tells us how much f will change if we move a little along the corresponding (akin to one-dim case)

- Conditions for optima defined similar to one-dim case
  - Required properties for one-dim case must be satisfied for all components of $\boldsymbol{x}$
- The second derivative in the multivariate case is known as the Hessian matrix

The Hessian

- For a multivar scalar valued function $f(\boldsymbol{x})$: $\mathbb{R}^D \rightarrow \mathbb{R}$, Hessian is a $D \times D$ matrix

$$\nabla^2 f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 x_D} \\ \frac{\partial^2 f}{\partial x_2 x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 x_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_D x_1} & \frac{\partial^2 f}{\partial x_D x_2} & \cdots & \frac{\partial^2 f}{\partial x_D^2} \end{bmatrix}$$

Gives information about the curvature of the function at point $\boldsymbol{x}$

Note: If the function itself is vector valued, e.g., $f(\boldsymbol{x})$: $\mathbb{R}^D \rightarrow \mathbb{R}^K$ then we will have K such $D \times D$ Hessian matrices, one for each output dimension of f

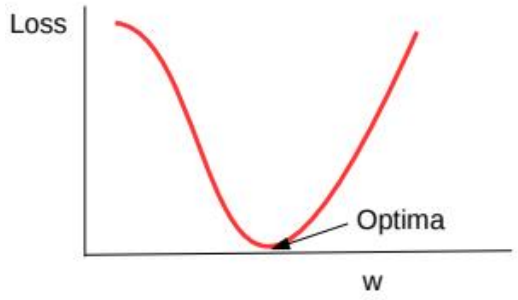
A square, symmetric $D \times D$ matrix M is PSD if $\boldsymbol{x}^\top M\boldsymbol{x} \geq \boldsymbol{0}\ \forall\ \boldsymbol{x} \in \mathbb{R}^D$
Will be NSD if $\boldsymbol{x}^\top M\boldsymbol{x} \leq \boldsymbol{0}\ \forall\ \boldsymbol{x} \in \mathbb{R}^D$

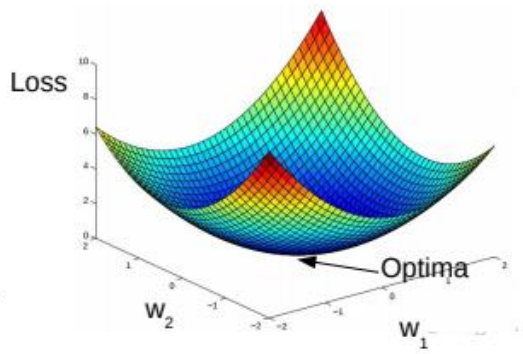
PSD if all eigenvalues are non-negative

- The Hessian matrix can be used to assess the optima/saddle points
  - $\nabla f(\boldsymbol{x}) = 0$ and $\nabla^2 f(\boldsymbol{x})$ is a positive semi-definite (PSD) matrix then $\boldsymbol{x}$ is a minima
  - $\nabla f(\boldsymbol{x}) = 0$, and $\nabla^2 f(\boldsymbol{x})$ is a negative semi-definite (NSD) matrix then $\boldsymbol{x}$ is a maxima
  - The determinant of the Hessian is zero at saddle point (has at least one zero eig-val)

Convex and Non-Convex Functions

- A function being optimized can be either convex or non-convex
- Here are a couple of examples of convex functions

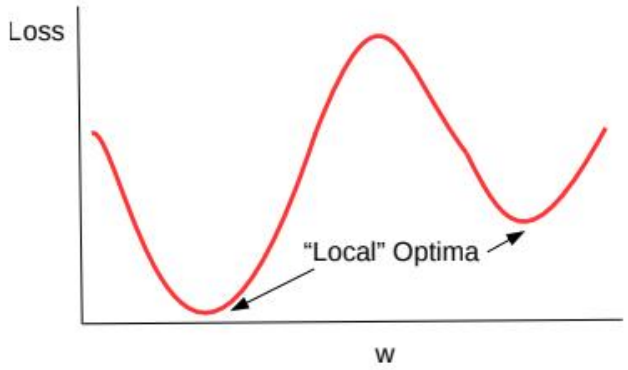


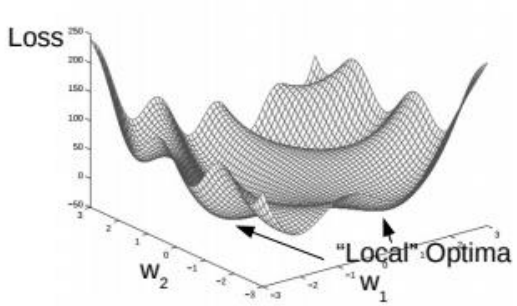


Convex functions are bowl-shaped. They have a unique optima (minima)

Negative of a convex function is called a concave function, which also has a unique optima (maxima)

- Here are a couple of examples of non-convex functions





Non-convex functions have multiple minima. Usually harder to optimize as compared to convex functions

Loss functions of most deep learning models are non-convex

Convex Sets

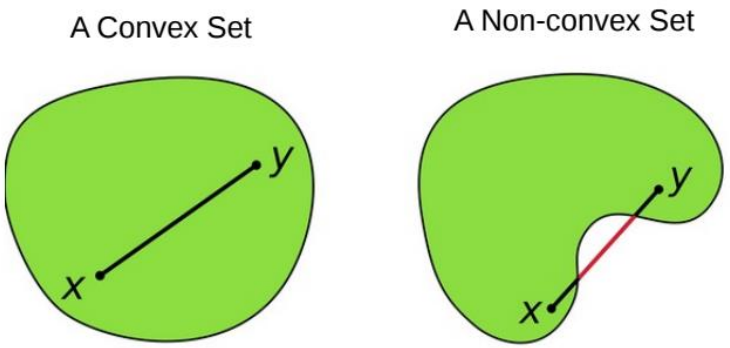
- A set S of points is a convex set, if for any two points $x, y \in S$, and $0 \leq \alpha \leq 1$

z is also called a "convex combination" of two points

$$z = \alpha x + (1 - \alpha) y \in S$$

Can also define convex combination of N points $x_1, x_2, \ldots, x_N$ as $z = \sum_{i=1}^{N} \alpha_i x_i$

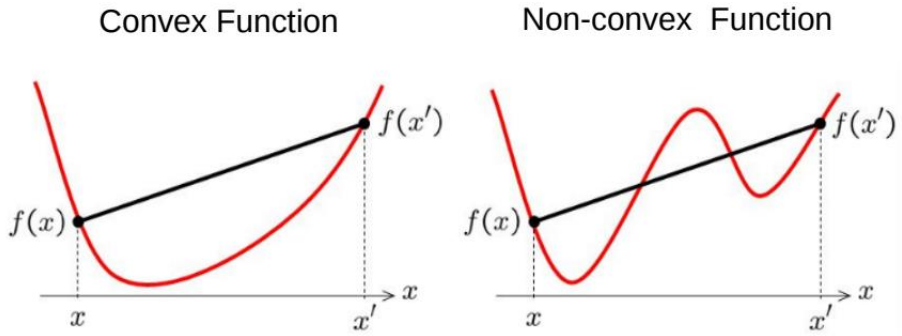
- Above means that all points on the line-segment between x and y lie within S



- The domain of a convex function needs to be a convex set

Convex Functions

- Informally, $f(x)$ is convex if all of its chords lie above the function everywhere



Note: "Chord lies above function" more formally means

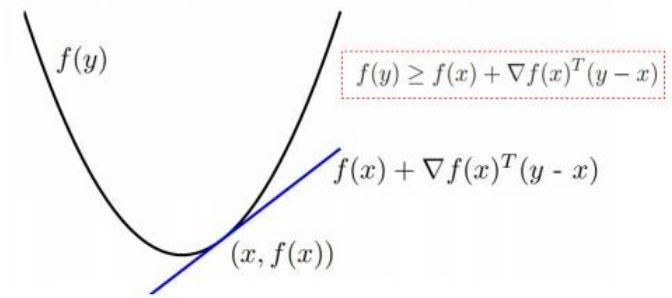
If f is convex then given

$$\alpha_1, \ldots, \alpha_n \text{ s.t } \sum_{i=1}^{n} \alpha_i = 1$$

$$f\left(\sum_{i=1}^{n} \alpha_i x_i\right) \leq \sum_{i=1}^{n} \alpha_i f(x_i)$$

Jensen's Inequality

- Formally, (assuming differentiable function), some tests for convexity:
  - First-order convexity (graph of f must be above all the tangents)



Exercise: Show that ridge regression objective is convex

  - Second derivative a.k.a. Hessian (if exists) must be positive semi-definite

Some Basic Rules for Convex Functions

- Some basic rules to check if $f(x)$ is convex or not
  - All linear and affine functions (e.g., $ax + b$) are convex
  - $\exp(ax)$ is convex for $x \in \mathbb{R}$, for any $a \in \mathbb{R}$
  - $\log(x)$ is concave (not convex) for $x > 0$
  - x^a is convex for $x > 0$, for any $a \geq 1$ and $a < 0$, concave for $0 \leq a \leq 1$
  - $|x|^a$ is convex for $x \in \mathbb{R}$, for any $a \geq 1$
  - All norms in $\mathbb{R}^D$ are convex
  - Non-negative weighted sum of convex functions is also a convex function
  - Affine transformation preserves convexity: if $f(x)$ is convex then $f(x) = f(ax + b)$ is also convex
  - Some rules to check whether composition $f(x) = h(g(x))$ of two functions h and g is convex

f is convex if h is convex and nondecreasing, and g is convex,
f is convex if h is convex and nonincreasing, and g is concave,
f is concave if h is concave and nondecreasing, and g is concave,
f is concave if h is concave and nonincreasing, and g is convex.

Optimization Problems in ML

- The general form of an optimization problem in ML will usually be

Usually a sum of the training error + regularizer

$$w_{opt} = \arg\min_{w \in C} L(w)$$

- Here $L(w)$ denotes the loss function to be optimized

- C is the constraint set that the solution must belong to, e.g.,
  - Non-negativity constraint: All entries in w_{opt} must be non-negative
  - Sparsity constraint: w_{opt} is a sparse vector with atmost K non-zeros

However, possible to have linear/ridge regression where solution has some constraints (e.g., non-neg, sparsity, or even both)

Linear and ridge regression that we saw were unconstrained (w_{opt} was a real-valued vector)

- If no C is specified, it is an unconstrained optimization problem

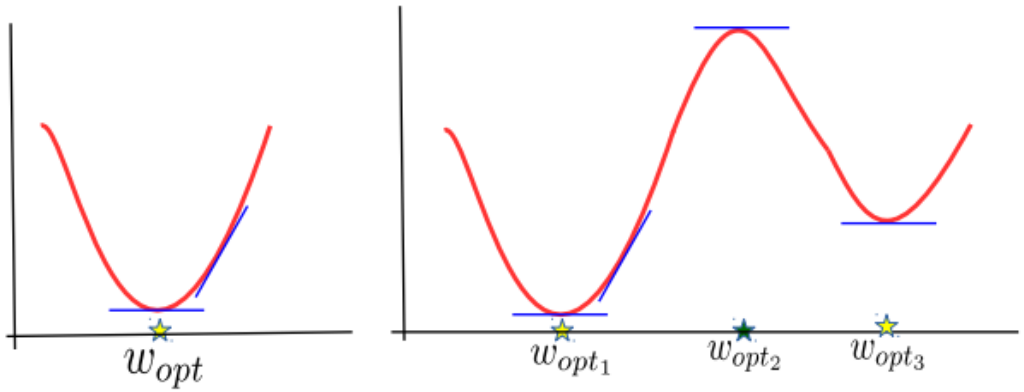
- Constrained opt. probs can be converted into unconstrained opt. (will see later)

- For now, assume we have an unconstrained optimization problem

Methods for Solving Optimization Problems

Method 1: Using First-Order Optimality

- Very simple. Already used this approach for linear and ridge regression



Called "first order" since only gradient is used and gradient provides the first order info about the function being optimized

The approach works only for very simple problems where the objective is convex and there are no constraints on the values $\boldsymbol{w}$ can take

- First order optimality: The gradient $\boldsymbol{g}$ must be equal to zero at the optima

$$\boldsymbol{g} = \nabla_{\boldsymbol{w}}[L(\boldsymbol{w})] = \mathbf{0}$$

- Sometimes, setting $\boldsymbol{g} = \mathbf{0}$ and solving for $\boldsymbol{w}$ gives a closed form solution

- If closed form solution is not available, the gradient vector $\boldsymbol{g}$ can still be used in iterative optimization algos, like gradient descent

Method 2: Iterative Optimiz. via Gradient Descent

Can I used this approach to solve maximization problems?

Fact: Gradient gives the direction of steepest change in function's value

For max. problems we can use gradient ascent

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \eta_t \boldsymbol{g}^{(t)}$$

Will move in the direction of the gradient

Iterative since it requires several steps/iterations to find the optimal solution

For convex functions, GD will converge to the global minima

Good initialization needed for non-convex functions

The learning rate very imp. Should be set carefully (fixed or chosen adaptively). Will discuss some strategies later

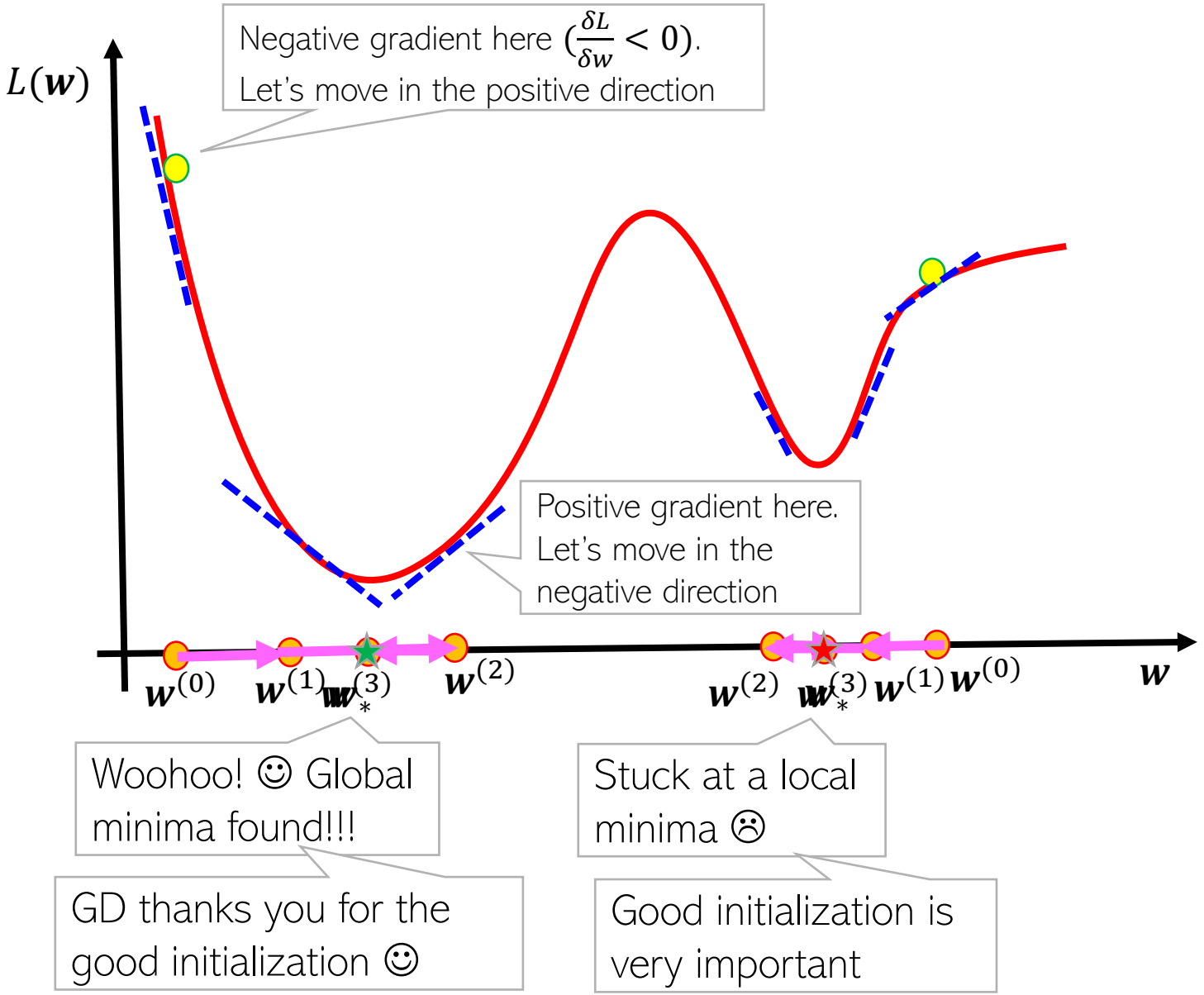
Gradient Descent

- Initialize $\boldsymbol{w}$ as $\boldsymbol{w}^{(0)}$
- For iteration $t = 0,1,2, \ldots$ (or until convergence)
  - Calculate the gradient $\boldsymbol{g}^{(t)}$ using the current iterates $\boldsymbol{w}^{(t)}$
  - Set the learning rate η_t
  - Move in the opposite direction of gradient

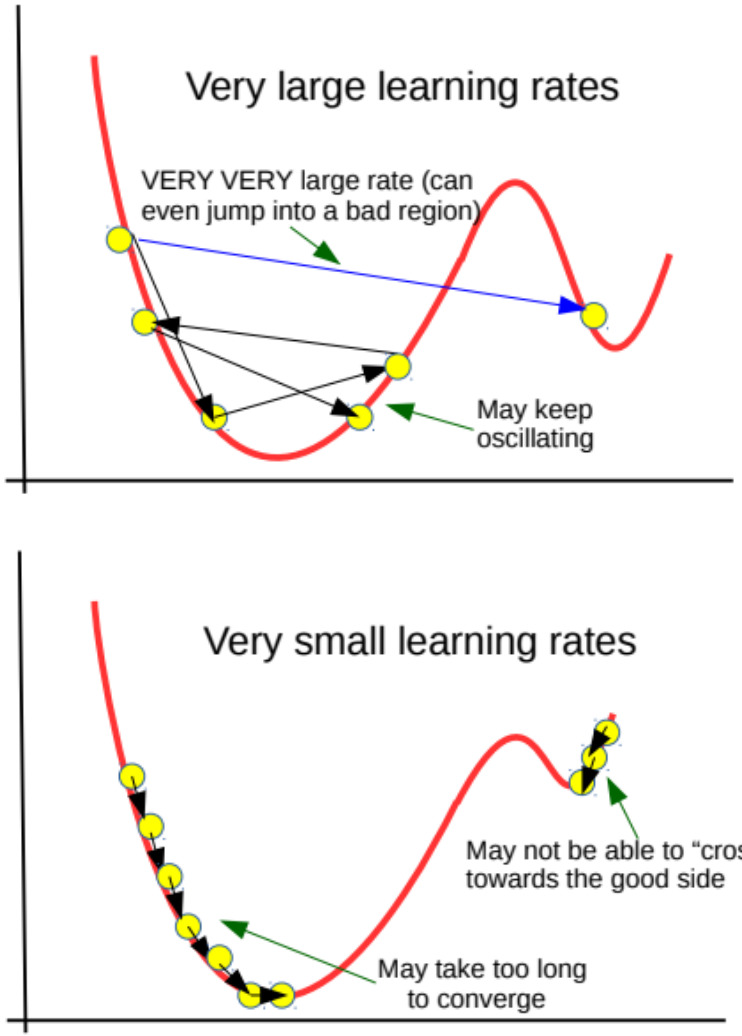
Will see the justification shortly

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta_t \boldsymbol{g}^{(t)}$$

Gradient Descent: An Illustration



Learning rate is very important



GD: An Example

- Let's apply GD for least squares linear regression

$$\boldsymbol{w}_{ridge} = \arg\min_{\boldsymbol{w}} L_{reg}(\boldsymbol{w}) = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

- The gradient: $\boldsymbol{g} = -\sum_{n=1}^{N} 2(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)\boldsymbol{x}_n$

- Each GD update will be of the form

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \eta_t \sum_{n=1}^{N} 2 \left(y_n - \boldsymbol{w}^{(t)\top} \boldsymbol{x}_n\right) \boldsymbol{x}_n$$

Prediction error of current model $\boldsymbol{w}^{(t)}$ on the n^{th} training example

Training examples on which the current model's error is large contribute more to the update

- Exercise: Assume $N = 1$, and show that GD update improves prediction on the training input $(\boldsymbol{x}_n, y_n)$, i.e, y_n is closer to $\boldsymbol{w}^{(t+1)\top} \boldsymbol{x}_n$ than to $\boldsymbol{w}^{(t)\top} \boldsymbol{x}_n$
  - This is sort of a proof that GD updates are "corrective" in nature (and it actually is true not just for linear regression but can also be shown for various other ML models)

Next class

- Optimizing non-differentiable functions
- Making GD faster: Stochastic gradient descent
- Constrained optimization
- Co-ordinate descent
- Alternating optimization
- Practical issue in optimization for ML