Optimization Techniques for ML (2)

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Introduction to Machine Learning (CS771A)

August 28, 2018

Recap: Convex and Non-Convex Function

- Most ML problems boil down to minimization of convex/non-convex functions, e.g.,

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \arg\min_{\boldsymbol{w}} \frac{1}{N}\sum_{n=1}^{N} \ell_n(\boldsymbol{w}) + R(\boldsymbol{w})$$

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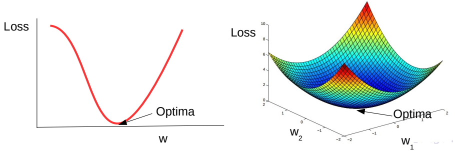

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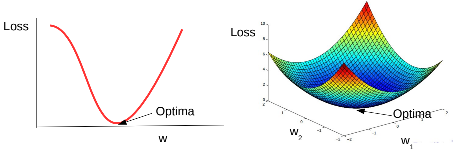
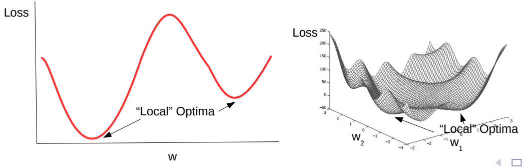


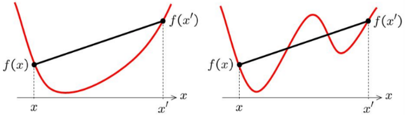
- Non-convex function have several local minima



Recap: Convex Functions

- A function is convex if all of its chords lie above the function

Convex Function Non-convex Function



Note: "Chord lies above function" more formally means

If f is convex then given

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

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

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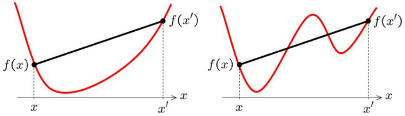

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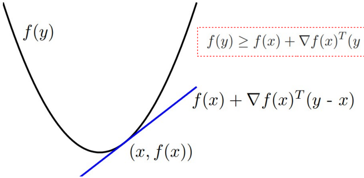

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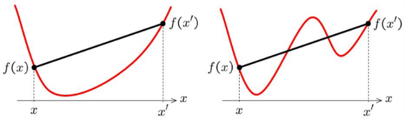

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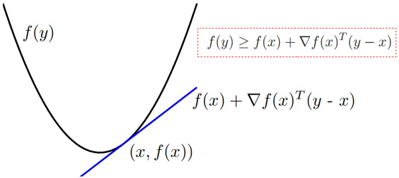

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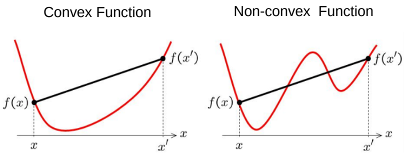

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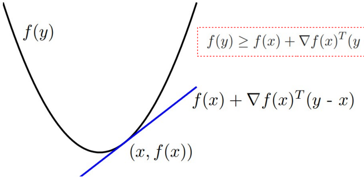
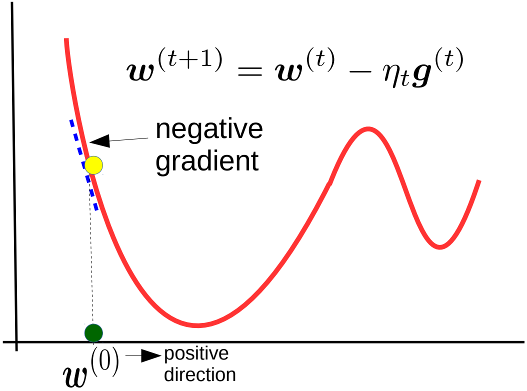


$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$

- A function is convex if its second derivative (Hessian) is positive semi-definite
- Note: If f is convex then $-f$ is a concave function

Recap: Gradient Descent

- A very simple, first-order method for optimizing any differentiable function (convex/non-convex)
- Uses only the gradient $\boldsymbol{g} = \nabla\mathcal{L}(\boldsymbol{w})$ of the function
- Basic idea: Start at some location $\boldsymbol{w}^{(0)}$ and move in the opposite direction of the gradient



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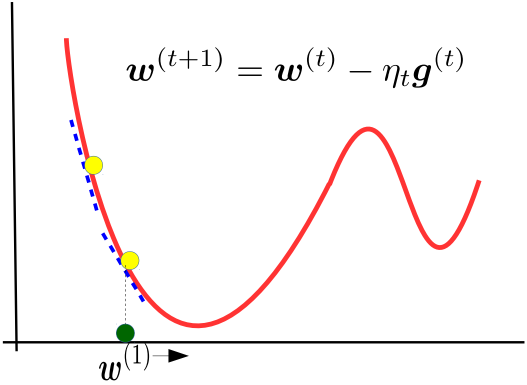

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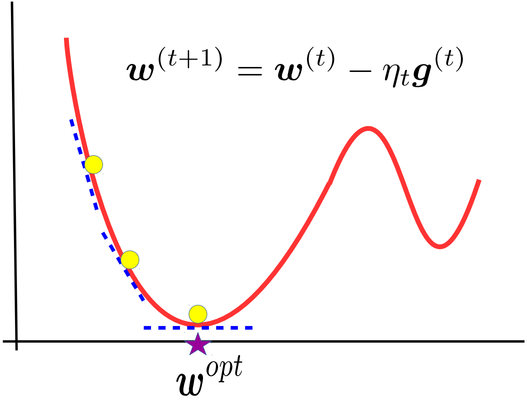

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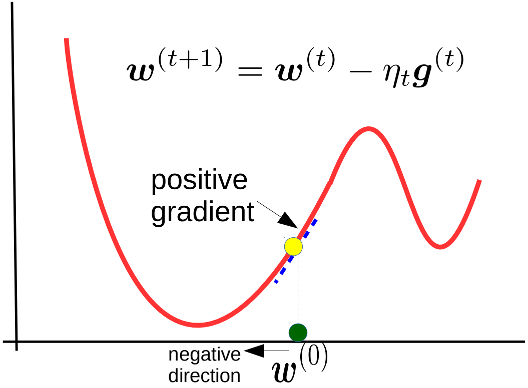

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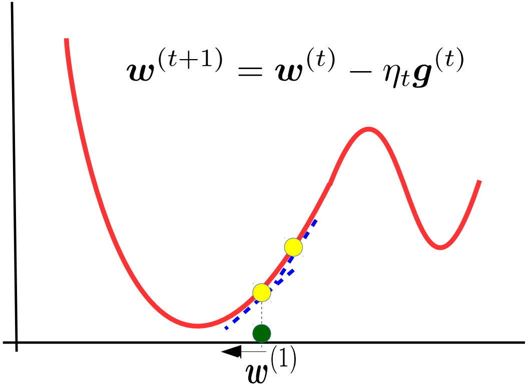

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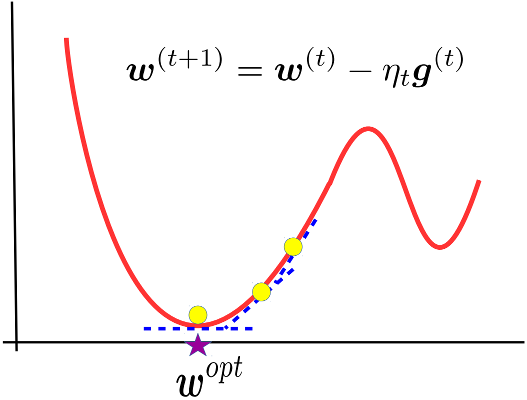

Gradient Descent

1. Initialize $\boldsymbol{w}$ as $\boldsymbol{w}^{(0)}$
2. Update $\boldsymbol{w}$ as follows

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

3. Repeat until convergence

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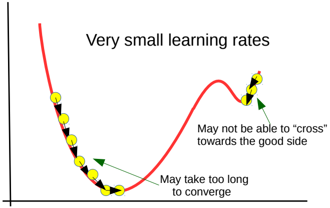
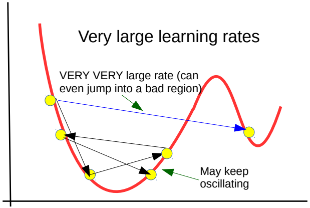
- The learning rate η_t is important
- Very small learning rates may result in very slow convergence
- Very large learning rates may lead to oscillatory behavior or result in a bad local optima





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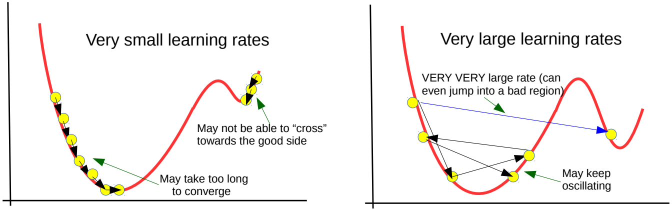

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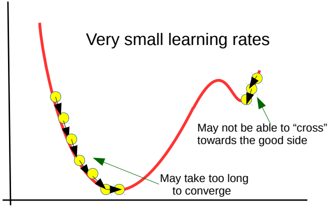

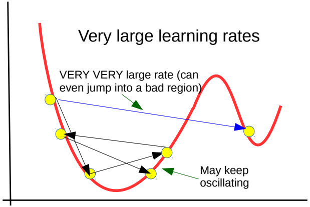

- Many ways to set the learning rate, e.g.,
  - Constant (if properly set, can still show good convergence behavior)
  - Decreasing with t (e.g. $1/t$, $1/\sqrt{t}$, etc.)
  - Use adaptive learning rates (e.g., using methods such as Adagrad, Adam)

Recap: Stochastic Gradient Descent

- Gradient computation in standard GD may be expensive when N is large

$$\boldsymbol{g} = \nabla_{\boldsymbol{w}} \left[\frac{1}{N} \sum_{n=1}^{N} \ell_n(\boldsymbol{w}) \right] = \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{g}_n \qquad \text{(ignoring regularizer } R(\boldsymbol{w})\text{)}$$

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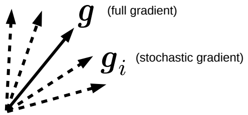

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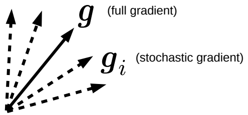

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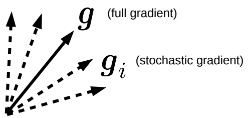

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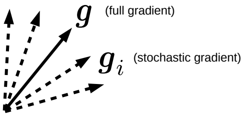

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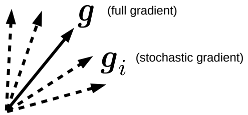

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- The algorithm is same as SGD except we will now using these mini-batch gradients at each step

Plan for today

- Optimization of functions that are NOT differentiable
- Optimization with constraints on the variables
- Optimizing w.r.t. several variables with one at a time
  - Co-ordinate descent
  - Alternating optimization
- Second-order methods for optimization

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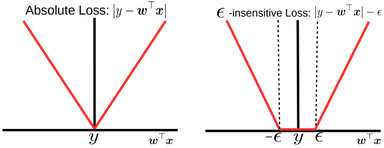
- Some common examples
  - Absolute, ϵ-insensitive loss in regression, several classification loss functions (we will see shortly)



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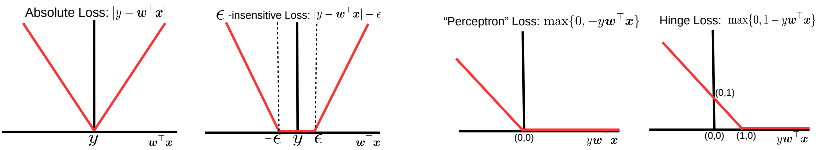

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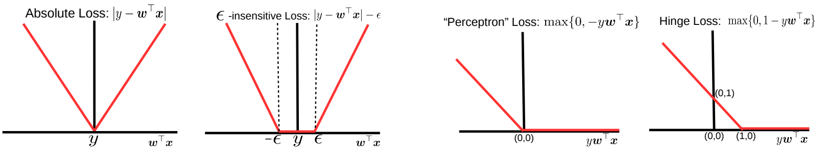

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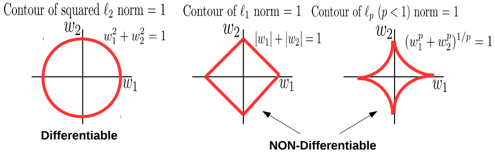

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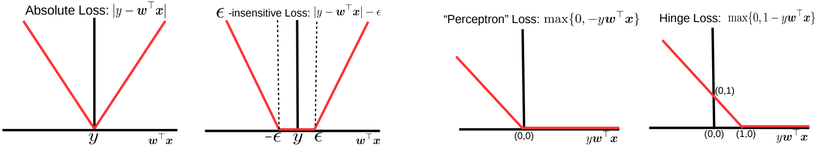

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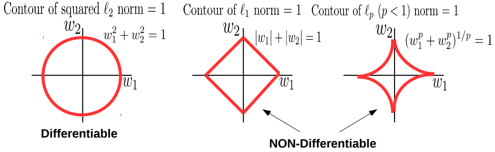

- Can't apply standard GD or SGD since gradient isn't defined at points of non-differentiability

Interlude: Loss Functions for Classification

- In regression (assuming linear model $\hat{y} = \boldsymbol{w}^\top \boldsymbol{x}$), some common loss functions are

$$\ell(y, \hat{y}) = (y - \boldsymbol{w}^\top \boldsymbol{x})^2 \quad \text{or} \quad \ell(y, \hat{y}) = |y - \boldsymbol{w}^\top \boldsymbol{x}|$$

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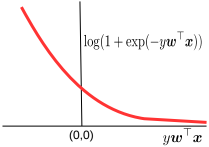
- Why does the above make sense? Well, it is large for large misclassifications, small otherwise



if y=+1, then large positive $\boldsymbol{w}^\top \boldsymbol{x}$ implies small error
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Large positive $y\boldsymbol{w}^\top \boldsymbol{x} \Rightarrow$ small error, Large negative $y\boldsymbol{w}^\top \boldsymbol{x} \Rightarrow$ large error

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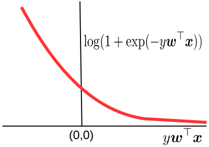
- In regression (assuming linear model $\hat{y} = \boldsymbol{w}^\top \boldsymbol{x}$), some common loss functions are

$$\ell(y, \hat{y}) = (y - \boldsymbol{w}^\top \boldsymbol{x})^2 \quad \text{or} \quad \ell(y, \hat{y}) = |y - \boldsymbol{w}^\top \boldsymbol{x}|$$

- We typically look at the difference between true y and model's prediction $\boldsymbol{w}^\top \boldsymbol{x}$
- How to formally define loss functions for classification?
- We have already looked at the loss function for logistic regression (assuming $y \in \{-1, +1\}$)

$$\ell(y, \hat{y}) = \log(1 + \exp(-y\boldsymbol{w}^\top \boldsymbol{x}))$$

- Why does the above make sense? Well, it is large for large misclassifications, small otherwise



if y=+1, then large positive $\boldsymbol{w}^\top \boldsymbol{x}$ implies small error

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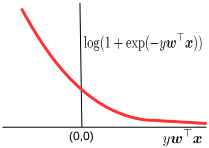

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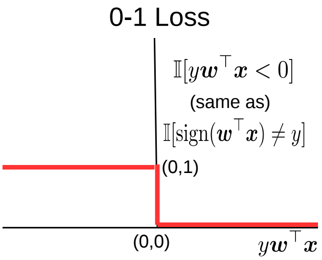
- Are there other loss functions for classification? Yes, several.

Interlude: Some Loss Functions for (Binary) Classification



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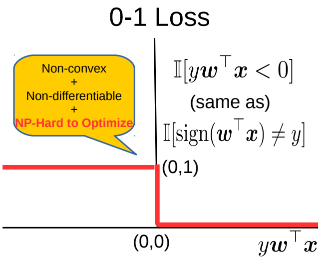

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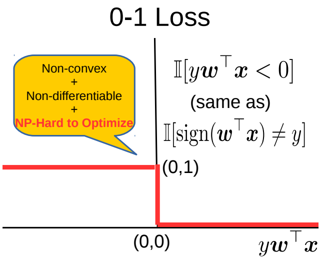

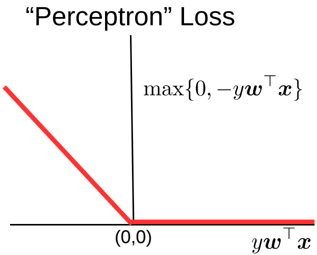

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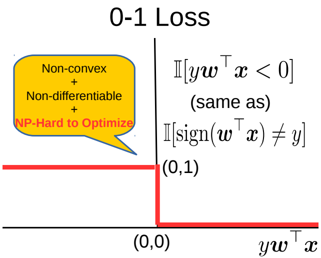

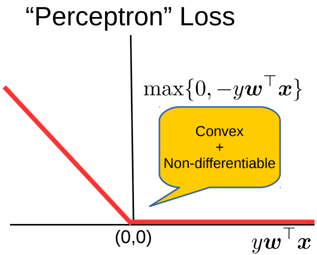

Interlude: Some Loss Functions for (Binary) Classification

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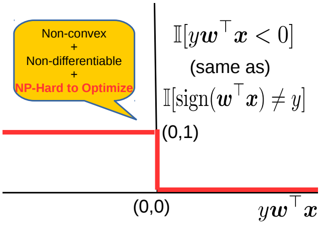
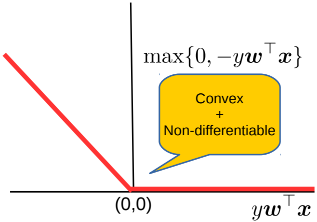
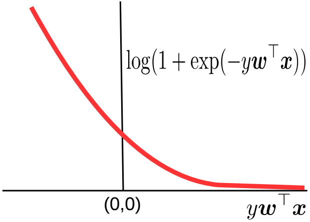


"Perceptron" Loss



Log(istic) Loss



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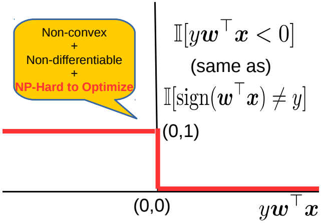

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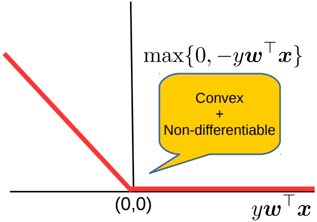

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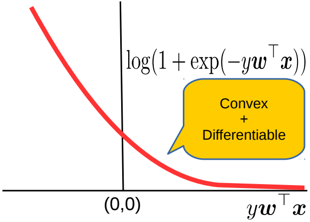

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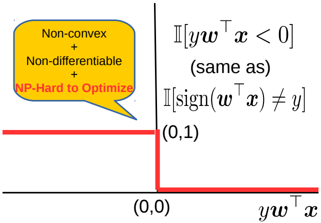

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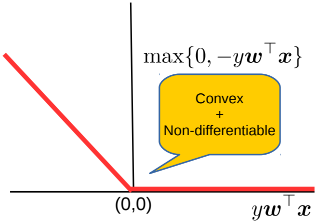

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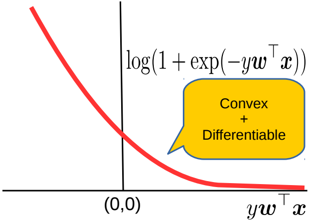
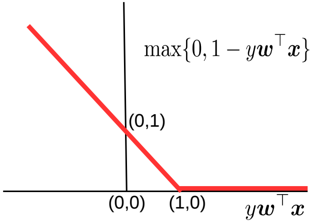


Hinge Loss



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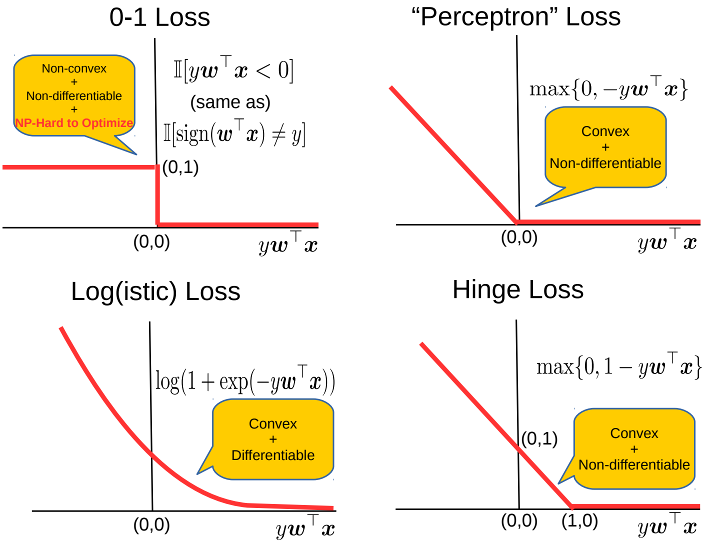
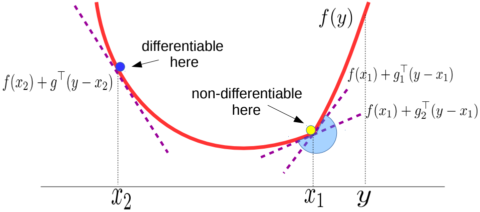


Optimizing Non-differentiable Functions

- Even though gradients are not defined for non-diff. functions, we can work with subgradients



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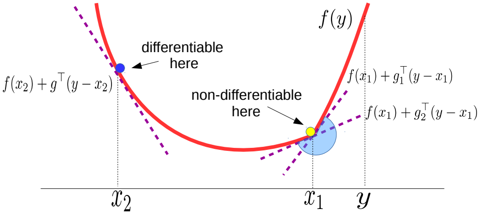

- For a function $f(\boldsymbol{x})$, its subgradient at $\boldsymbol{x}$ is <u>any</u> vector $\boldsymbol{g}$ s.t. $\forall \boldsymbol{y}$

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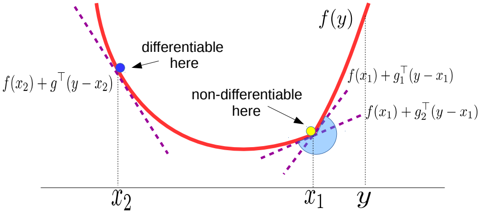

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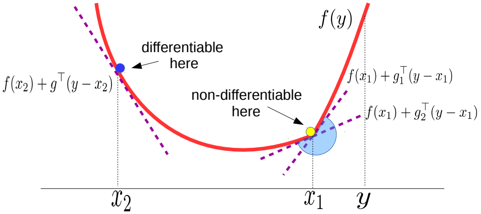

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- A non-differentiable function can have several subgradients at the point of non-differentiability
- Set of all subgradients of a function f at point $\boldsymbol{x}$ is called the subdifferential denoted as $\partial f(\boldsymbol{x})$

$$\partial f(\boldsymbol{x}) = \{\boldsymbol{g} : f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{g}^\top (\boldsymbol{y} - \boldsymbol{x}), \quad \forall \boldsymbol{y}\}$$

Subgradient Descent: An Example

- Consider linear regression but with ℓ_1 norm on $\boldsymbol{w}$ (recall: ℓ_1 norm promotes a sparse $\boldsymbol{w}$)

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \lambda ||\boldsymbol{w}||_1$$

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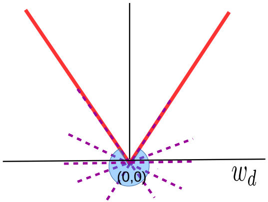
- Here $\boldsymbol{t}$ is a vector s.t.

$$t_d = \begin{cases} -1, & \text{for } w_d < 0 \\ [-1, +1] & \text{for } w_d = 0 \\ +1 & \text{for } w_d > 0 \end{cases}$$



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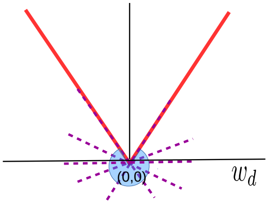
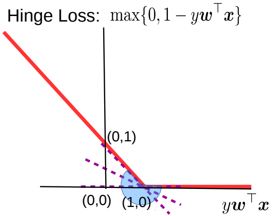


- If we take $t_d = 0$ at $w_d = 0$ then $t_d = \text{sign}(w_d)$

Subgradient Descent: Another Example

- Consider binary classification with hinge loss (used in SVM - will see later), assume ℓ_2 regularizer



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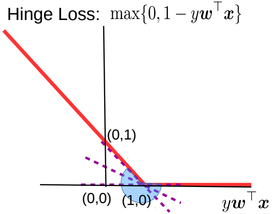
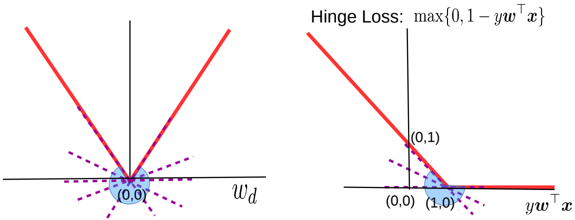


- In this case loss (hinge) non-differentiable, regularizer differentiable
- Subgradient $\boldsymbol{t}$ of the hinge loss term will be

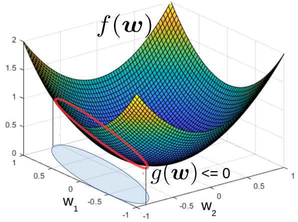
$$\boldsymbol{t} = \begin{cases} 0, & \text{for } y_n \boldsymbol{w}^\top \boldsymbol{x}_n > 1 \\ -y_n \boldsymbol{x}_n & \text{for } y_n \boldsymbol{w}^\top \boldsymbol{x}_n < 1 \\ k y_n \boldsymbol{x}_n & \text{for } y_n \boldsymbol{w}^\top \boldsymbol{x}_n = 1 \quad (\text{where } k \in [-1, 0]) \end{cases}$$

Subgradient Descent: Summary



- Not really that different from standard GD
- Only difference is that we use subgradients where function is non-differentiable
- In practice, it is like pretending that the function is differentiable everywhere

Constrained Optimization



1: Lagrangian based optimization

2: Projected gradient descent

Constrained Optimization: Lagrangian Approach

- Consider optimizing some function $f(\mathbf{w})$ subject to an inequality constraint on $\mathbf{w}$

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} f(\mathbf{w}), \quad \text{s.t.} \quad g(\mathbf{w}) \leq 0$$

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- Primal and Dual problems

$$\hat{\boldsymbol{w}}_P = \arg\min_{\boldsymbol{w}} \left\{ \arg\max_{\alpha \geq 0} \{ f(\boldsymbol{w}) + \alpha g(\boldsymbol{w}) \} \right\} \qquad \text{(primal problem)}$$

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- For dual solution, $\alpha_D g(\hat{\mathbf{w}}_D) = 0$ (complimentary slackness/Karush-Kuhn-Tucker (KKT) condition)

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Lagrangian based Optimization: An Example

- Consider the generative classification model with K classes
- Suppose we want to estimate the parameters of class-marginal $p(y)$

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- Exercise: Solve $\arg\max_{\beta} \arg\min_{\boldsymbol{\pi}} \mathcal{L}(\boldsymbol{\pi}, \beta)$ and show that $\pi_k = N_k/N$

Projected Gradient Descent

- Suppose our problem requires the parameters to lie within a set $\mathcal{C}$

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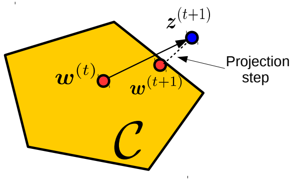

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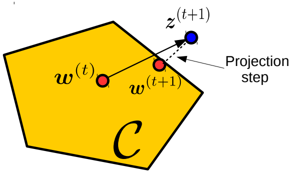
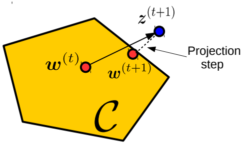


- Each step of projected GD works as follows
  - Do the usual GD update: $\boldsymbol{z}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta_t \boldsymbol{g}^{(t)}$
  - Check $\boldsymbol{z}^{(t+1)}$ for the constraints
    - If $\boldsymbol{z}^{(t+1)} \in \mathcal{C}$, $\boldsymbol{w}^{(t+1)} = \boldsymbol{z}^{(t+1)}$
    - If $\boldsymbol{z}^{(t+1)} \notin \mathcal{C}$, project on the constraint set: $\boldsymbol{w}^{(t+1)} = \underbrace{\Pi_{\mathcal{C}}[\boldsymbol{z}^{(t+1)}]}_{\text{projection}}$

Projected GD: How to Project?

- The projection itself is an optimization problem



- Given $\boldsymbol{z}$, we find the "closest" point (e.g., in Euclidean sense) $\boldsymbol{w}$ in the set as follows

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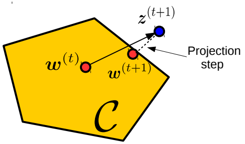

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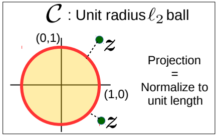

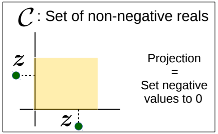

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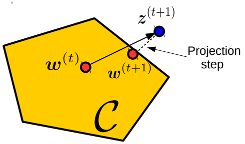

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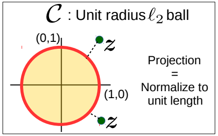

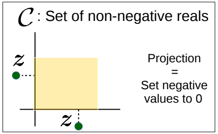

- For some other sets $\mathcal{C}$, the projection step may be a bit more involved

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    - $t = t + 1$. Repeat until convergence

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Alternating Optimization

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- For simplicity, suppose we want to optimize a function of 2 variables $\boldsymbol{w}_1 \in \mathbb{R}^D$ and $\boldsymbol{w}_2 \in \mathbb{R}^D$

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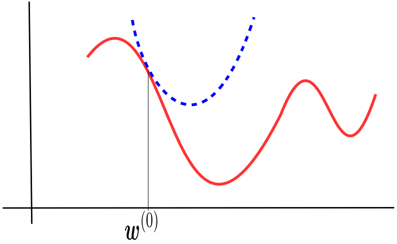

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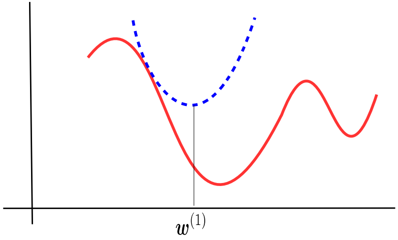

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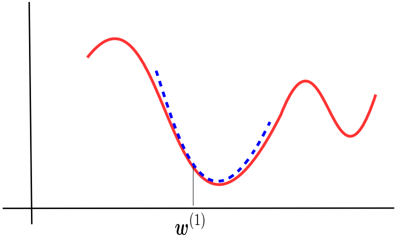

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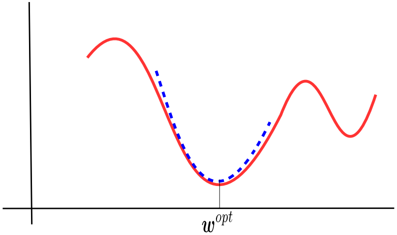

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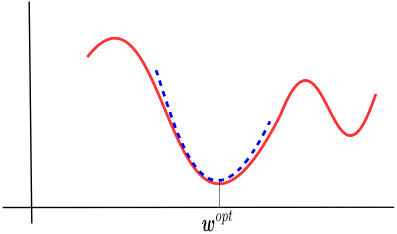

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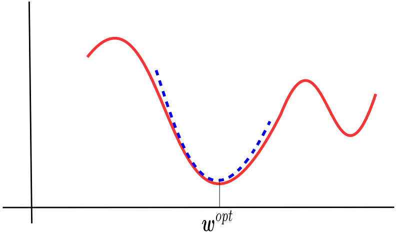

- Doesn't rely on gradient to choose $\boldsymbol{w}^{(t+1)}$
- Instead, each step directly jumps to the minima of quadratic approximation

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- Many ways to approximate the Hessian (e.g., using previous gradients); also look at L-BFGS etc.

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- Gradient methods are simple to understand and implement
- More sophisticated optimization methods often use gradient methods
  - Backpropagation algorithm used in deep neural nets is GD + chain rule of differentiation
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  - But having a good understanding of optimization is still helpful