# Optimization for ML (contd)

CS771: Introduction to Machine Learning

#### Plan today

- Optimization methods
  - Stochastic gradient descent
  - Co-ordinate descent
  - Alternating optimization
  - Second order optimization
  - Some practical aspects
  - Constrained optimization
    - Projected gradient descent
    - Lagrangian based method
  - Optimization of non-differentiable functions
    - Subgradient descent



#### Faster GD: Stochastic Gradient Descent (SGD)

- lacktriangle Consider a loss function of the form  $L(oldsymbol{w}) = rac{1}{N} \sum_{n=1}^N \ell_n(oldsymbol{w})$
- Writing as an average instead of sum. Won't affect minimization of L(w)

■ The gradient in this case can be written as

Expensive to compute – requires doing it for all the training examples in each iteration  $\otimes$ 

$$\boldsymbol{g} = \nabla_{\boldsymbol{w}} L(\boldsymbol{w}) = \nabla_{\boldsymbol{w}} \left[ \frac{1}{N} \sum_{n=1}^{N} \ell_n(\boldsymbol{w}) \right] = \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{g}_n$$
Gradient of the loss on  $n^{th}$  training example

- ullet Stochastic Gradient Descent (SGD) approximates  $oldsymbol{g}$  using a <u>single</u> training example
- At iter. t, pick an index  $i \in \{1,2,...,N\}$  uniformly randomly and approximate g as

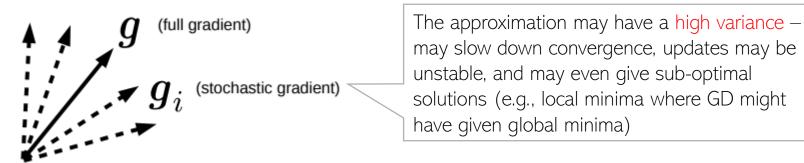
$$\boldsymbol{g} \approx \boldsymbol{g}_i = \nabla_{\boldsymbol{w}} \ell_i(\boldsymbol{w})$$

Can show that  $g_i$  is an unbiased estimate of g, i.e.,  $\mathbb{E}[g_i] = g$ 

- May take more iterations than GD to converge but each iteration is much faster ©
  - SGD per iter cost is O(D) whereas GD per iter cost is O(ND)

#### Minibatch SGD

Gradient approximation using a single training example may be noisy



- We can use B>1 unif. rand. chosen train. ex. with indices  $\{i_1,i_2,\ldots,i_B\}\in\{1,2,\ldots,N\}$
- Using this "minibatch" of examples, we can compute a minibatch gradient

$$\boldsymbol{g} \approx \frac{1}{B} \sum_{b=1}^{B} \boldsymbol{g}_{i_b}$$

- Averaging helps in reducing the variance in the stochastic gradient
- Time complexity is O(BD) per iteration in this case



### Some Practical Aspects: Iterate Averaging for SGD

■ SGD iterates  $w^{(1)}$ ,  $w^{(2)}$ ,  $w^{(3)}$ , ... can be noisy (recall SGD computes gradients using randomly picked single training example, or a small minibatch)

Polyak-Ruppert Averaging: Average SGD iterates and use the average in the end

SGD/mini-batch SGD update at iteration t+1  $w^{(t+1)} = w^{(t)} - \eta_t g^{(t)}$ Running average weight vector at iteration t+1Running average weight vector at previous iteration t t t t t t

This way of computing the average is the same as doing  $\overline{\boldsymbol{w}}^{(t+1)} = \sum_{i=1}^{t+1} \boldsymbol{w}^{(i)}$  but to avoid storing the previous weights, so we compute a running average

Sometimes, we don't start averaging from iteration 1 but after some warm-up iterations

 $\frac{1}{1}w^{(t+1)}$ 

Averaging is quite popular for SGD. Stochastic Weighted Averaging (SWA) is another such recently proposed scheme (similar to Polyak-Ruppert Averaging) used for deep neural networks

#### Co-ordinate Descent (CD)

- Standard gradient descent update for :  $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} \eta_t \mathbf{q}^{(t)}$
- $\blacksquare$  CD: In each iter, update only one entry (co-ordinate) of  $\boldsymbol{w}$ . Keep all others fixed

$$w_d^{(t+1)} = w_d^{(t)} - \eta_t g_d^{(t)} \qquad d \in \{1,2,\dots,D\}$$
 
$$w_d^{(t+1)} = w_d^{(t+1)} - \eta_t g_d^{(t)} \qquad d \in \{1,2,\dots,D\}$$
 te i ow independent of  $D$ 

- Cost of each update i
- pdate unif. randd In each iter, can choos co-ordinate to y or in cyclic order
- ngle co-ord, can also <u>up</u>date "pp s" of co-ordinates Instead of updating a
  - descent (BCD) Called block co-ordina
- To avoid O(D) cost o radient compution, can cache evious computations
  - ations may have ms like  $w^{\mathsf{T}}x$  if j one co-ordinate of w Recall that grad. comp changes, we should a domputing the  $\mathbf{w}^{\mathsf{T}}\mathbf{x}$  (=  $\sum_{d} w_{d}$ from scratch

#### Alternating Optimization (ALT-OPT)

Each variable can be scalar or vector or matrix or tensor

lacktriangleright Consider opt. problems with several variables, say two variables  $oldsymbol{w_1}$  and  $oldsymbol{w_2}$ 

$$\{\hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2\} = \arg\min_{\boldsymbol{w}_1, \boldsymbol{w}_2} \mathcal{L}(\boldsymbol{w}_1, \boldsymbol{w}_2)$$

E.g. first order optimality doesn't give a closed form solution when solving for both variables jointly

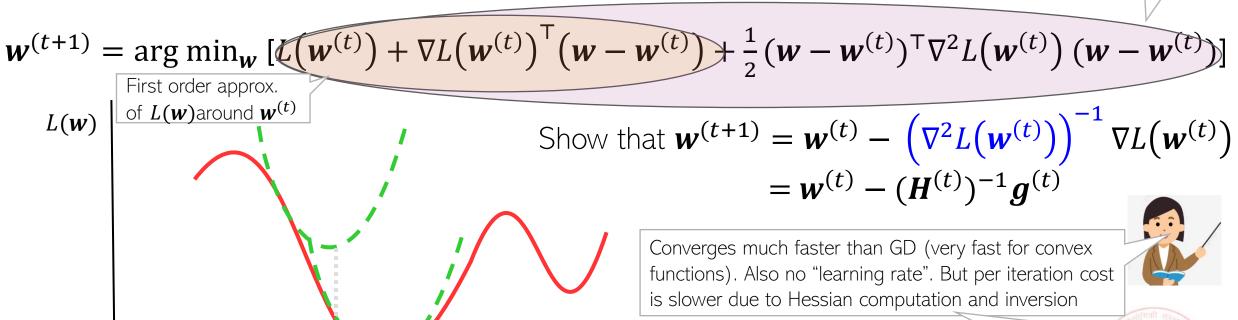
- Often, this "joint" optimization is hard/impossible to solve
- We can take an alternating optimization approach to solve such problems

#### **ALT-OPT**

- 1 Initialize one of the variables, e.g.,  $\mathbf{w}_2 = \mathbf{w}_2^{(0)}, t = 0$
- Solve  $\mathbf{w}_1^{(t+1)} = \arg\min_{\mathbf{w}_1} \mathcal{L}(\mathbf{w}_1, \mathbf{w}_2^{(t)})$  // $\mathbf{w}_2$  "fixed" at its most recent value  $\mathbf{w}_2^{(t)}$
- Solve  $\mathbf{w}_2^{(t+1)} = \arg\min_{\mathbf{w}_2} \mathcal{L}(\mathbf{w}_1^{(t+1)}, \mathbf{w}_2)$  // $\mathbf{w}_1$  "fixed" at its most recent value  $\mathbf{w}_1^{(t+1)}$
- t = t + 1. Go to step 2 if not converged yet.
- Usually converges to a local optima. But very very useful. Will see examples later
  - Also related to the Expectation-Maximization (EM) algorithm which we will see later CS771: Intro to ML

#### Second Order Methods: Newton's Method

- Unlike GD and its variants, Newton's method uses second-order information (second derivative, a.k.a. the Hessian). Iterative method, just like GD
- lacktriangle Given current  $oldsymbol{w}^{(t)}$ , minimize the quadratic (second-order) approx. of  $\overline{L(oldsymbol{w})}$



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Faster versions of Newton's method also exist, e.g.,

gradients (see L-BFGS which is a popular method)

those based on approximating Hessian using previous

#### Some Practical Aspects: Assessing Convergence

- Various ways to assess convergence, e.g. consider converged if
  - The objective's value (on train set) ceases to change much across iterations

$$L(\boldsymbol{w}^{(t+1)})$$
 -  $L(\boldsymbol{w}^{(t)}) < \epsilon$  (for some small pre-defined  $\epsilon$ )

■ The parameter values cease to change much across iterations

$$\| \boldsymbol{w}^{(t+1)} - \boldsymbol{w}^{(t)} \| < \tau$$
 (for some small pre-defined  $\tau$ )

Above condition is also equivalent to saying that the gradients are close to zero

$$\|\boldsymbol{g}^{(t)}\| \to 0$$

Caution: May not yet be at the optima. Use at your own risk!

- The objective's value has become small enough that we are happy with ②
- Use a validation set to assess if the model's performance is acceptable (early stopping)

## Some Practical Aspects: Learning Rate (Step Size)

lacktriangle Some guidelines to select good learning rate (a.k.a. step size)  $\eta_t$ 

C is a hyperparameter

- For convex functions, setting  $\eta_t$  something like C/t or  $C/\sqrt{t}$  often works well
  - These step-sizes are actually theoretically optimal in some settings. Moreover we want
    - $\eta_t \to 0$  as t becomes very very large
    - $\blacksquare \sum \eta_t = \infty$  (needed to ensure that we can potentially reach anywhere in the parameter space)
    - $\sum {\eta_t}^2 < \infty$  (to prevent indefinite oscillatory behavior around the optima)
  - Sometimes carefully chosen constant learning rates (usually small, or initially large and later small) also work well in practice
- Can also search for the "best" step-size by solving an opt. problem in each step

Also called "line search" 
$$\eta_t = \arg\min_{\eta \geq 0} f(\mathbf{w}^{(t)} - \eta \cdot \mathbf{g}^{(t)})$$
 A one-dim optimization problem (note that  $\mathbf{w}^{(t)}$  and  $\mathbf{g}^{(t)}$  are fixed)

- A faster alternative to line search is the Armijo-Goldstein rule
  - Starting with current (or some large) learning rate (from prev. iter), and try a few values in decreasing order until the objective's value has a sufficient reduction

## Some Practical Aspects: Adaptive Gradient Methods

Can also use different learning rate in different dimensions

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \boldsymbol{e}^{(t)} \odot \boldsymbol{g}^{(t)} \qquad e_d^{(t)} = \frac{1}{\sqrt{\epsilon + \sum_{\tau=1}^t \left(g_d^{(\tau)}\right)^2}}$$
Vector of learning rates along each dimension two vectors

If some dimension had big updates recently (marked by large gradient values), slow down along those directions by using smaller learning rates - AdaGrad (Duchi et al, 2011)

- Can use a momentum term to stabilize gradients by reusing info from past grads
  - Move faster along directions that were <u>previously</u> good
  - Slow down along directions where gradient has <u>changed abruptly</u>

 $oldsymbol{eta}$  usually set as 0.9

The "momentum" term.
Set to 0 at initialization

$$\boldsymbol{m}^{(t)} = \beta \boldsymbol{m}^{(t-1)} + (1 - \beta) \boldsymbol{g}^{(t)}$$
$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \boldsymbol{m}^{(t)}$$

In an even faster version of this,  $\mathbf{g}^{(t)} = \nabla L(\mathbf{w}^{(t)})$  is replaced by the gradient computed at the next step if previous direction were used, i.e.,  $\nabla L(\mathbf{w}^{(t)} - \beta \mathbf{m}^{(t-1)})$ . Called Nesterov's Accelerated Gradient (NAG) method

- Also exist several more advanced methods that combine the above methods
  - RMS-Prop: AdaGrad + Momentum, Adam: NAG + RMS-Prop
  - These methods are part of packages such as PyTorch, Tensorflow, etc

# Constrained Optimization



#### Projected Gradient Descent

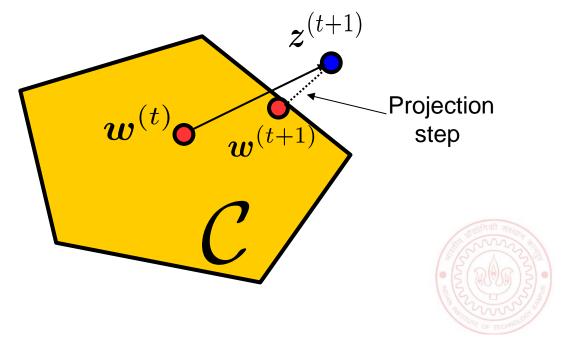
Consider an optimization problem of the form

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

Projection

operator

- Projected GD is very similar to GD with an extra projection step
- Each iteration t will be of the form
  - Perform update:  $\mathbf{z}^{(t+1)} = \mathbf{w}^{(t)} \eta_t \mathbf{g}^{(t)}$
  - Check if  $z^{(t+1)}$  satisfies constraints
    - If  $\mathbf{z}^{(t+1)} \in \mathcal{C}$ , set  $\mathbf{w}^{(t+1)} = \mathbf{z}^{(t+1)}$
    - If  $\mathbf{z}^{(t+1)} \notin \mathcal{C}$ , project as  $\mathbf{w}^{(t+1)} = \Pi_{\mathcal{C}}[\mathbf{z}^{(t+1)}]$



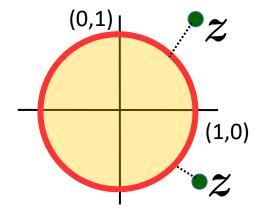
#### Projected GD: How to Project?

■ Here projecting a point means finding the "closest" point from the constraint set

$$\Pi_{\mathcal{C}}[\mathbf{z}] = \arg\min_{\mathbf{w} \in \mathcal{C}} \|\mathbf{z} - \mathbf{w}\|^{2}$$

lacktriangle For some sets  $\mathcal{C}$ , the projection step is easy

 ${\cal C}$ : Unit radius  $\ell_2$  ball



Projection = Normalize to unit Euclidean length vector

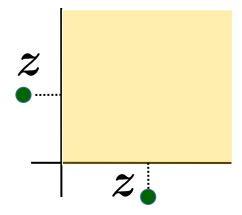
$$\hat{\mathbf{x}} = \begin{cases} \mathbf{x} & \text{if } \|\mathbf{x}\|_2 \le 1\\ \frac{\mathbf{x}}{\|\mathbf{x}\|_2} & \text{if } \|\mathbf{x}\|_2 > 1 \end{cases}$$

Another constrainted optimization problem! But simpler to solve! ©

Projected GD commonly used only when the projection step is simple and efficient to compute



 ${\cal C}$ : Set of non-negative reals



Projection = Set each negative entry in z to be zero

$$\hat{\mathbf{x}}_i = \begin{cases} \mathbf{x}_i & \text{if } \mathbf{x}_i \ge 0\\ 0 & \text{if } \mathbf{x}_i < 0 \end{cases}$$

#### Constrained Opt. via Lagrangian

lacktriangle Consider the following constrained minimization problem (using f instead of L)

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

- Note: If constraints of the form  $g(w) \ge 0$ , use  $-g(w) \le 0$
- Can handle multiple inequality and equality constraints too (will see later)
- Can transform the above into the following equivalent <u>unconstrained</u> problem

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} f(\boldsymbol{w}) + c(\boldsymbol{w})$$

$$c(\mathbf{w}) = \max_{\alpha \ge 0} \alpha g(\mathbf{w}) = \begin{cases} \infty, & \text{if } g(\mathbf{w}) > 0 \\ 0 & \text{if } g(\mathbf{w}) \le 0 \end{cases} \text{ (constraint violated)}$$

Our problem can now be written as

$$\widehat{\mathbf{w}} = \arg\min_{\mathbf{w}} \left\{ f(\mathbf{w}) + \max_{\alpha \ge 0} \alpha g(\mathbf{w}) \right\}$$

#### Constrained Opt. via Lagrangian

The Lagrangian:  $\mathcal{L}(w, \alpha)$ 

■ Therefore, we can write our original problem as

$$\widehat{\mathbf{w}} = \arg\min_{\mathbf{w}} \left\{ f(\mathbf{w}) + \max_{\alpha \ge 0} \alpha g(\mathbf{w}) \right\} = \arg\min_{\mathbf{w}} \left\{ \max_{\alpha \ge 0} \left\{ f(\mathbf{w}) + \alpha g(\mathbf{w}) \right\} \right\}$$

- The Lagrangian is now optimized w.r.t.  $m{w}$  and  $m{lpha}$  (Lagrange multiplier)
- We can define Primal and Dual problem as

$$\widehat{\boldsymbol{w}}_{P} = \arg\min_{\boldsymbol{w}} \left\{ \max_{\alpha \geq 0} \left\{ f(\boldsymbol{w}) + \alpha g(\boldsymbol{w}) \right\} \right\}$$
 (Primal Problem)
$$\widehat{\boldsymbol{w}}_{D} = \arg\max_{\alpha \geq 0} \left\{ \min_{\boldsymbol{w}} \left\{ f(\boldsymbol{w}) + \alpha g(\boldsymbol{w}) \right\} \right\}$$
 (Dual Problem)

Both equal if f(w) and the set  $g(w) \le 0$  are convex

$$\alpha_D g(\hat{\mathbf{w}}_D) = 0$$

complimentary slackness/Karush-Kuhn-Tucker (KKT) condition

#### Constrained Opt. with Multiple Constraints

We can also have multiple inequality and <u>equality</u> constraints

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} f(\boldsymbol{w})$$
  
s.t.  $g_i(\boldsymbol{w}) \leq 0, \quad i = 1, ..., K$   
 $h_j(\boldsymbol{w}) = 0, \quad j = 1, ..., L$ 

- lacktriangle Introduce Lagrange multipliers  $m{lpha}=[lpha_1,lpha_2,...,lpha_K]$  and  $m{eta}=[eta_1,eta_2,...,eta_L]$
- The Lagrangian based primal and dual problems will be

$$\widehat{\boldsymbol{w}}_{P} = \arg\min_{\boldsymbol{w}} \left\{ \max_{\alpha \geq 0, \beta} \left\{ f(\boldsymbol{w}) + \sum_{i=1}^{K} \alpha_{i} g_{i}(\boldsymbol{w}) + \sum_{j=1}^{L} \beta_{j} h_{j}(\boldsymbol{w}) \right\} \right\}$$

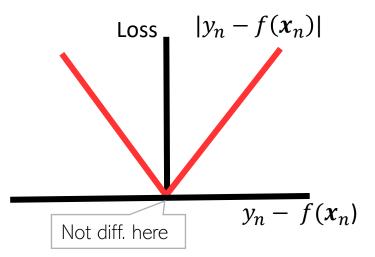
$$\widehat{\boldsymbol{w}}_{D} = \arg\max_{\alpha \geq 0, \beta} \left\{ \min_{\boldsymbol{w}} \left\{ f(\boldsymbol{w}) + \sum_{i=1}^{K} \alpha_{i} g_{i}(\boldsymbol{w}) + \sum_{j=1}^{L} \beta_{j} h_{j}(\boldsymbol{w}) \right\} \right\}_{\text{CS771: Intro to N}}$$

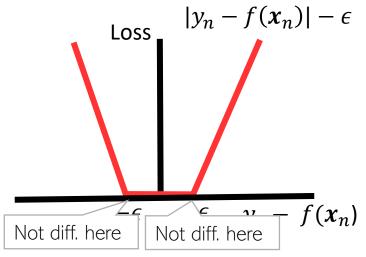
# Optimization of Non-differentiable Functions



#### Dealing with Non-differentiable Functions

- In many ML problems, the objective function will be non-differentiable
- Some examples that we have already seen: Linear regression with absolute loss, or  $\epsilon$ -insensitive loss; even  $\ell_1$  norm regularizer is non-diff



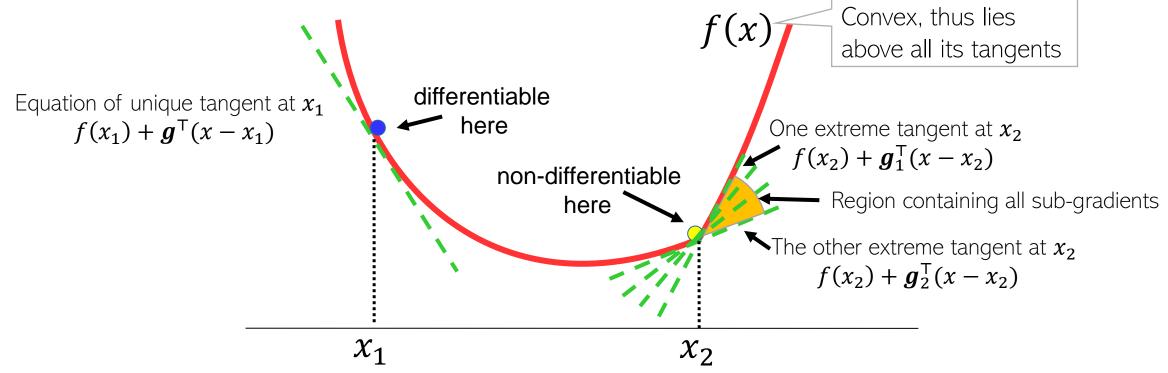


- Basically, any function in which there are points with kink is non-diff
  - At such points, the function is non-differentiable and thus gradients not defined
  - Reason: Can't define a unique tangent at such points



#### Sub-gradients

■ For convex non-diff fn, can define sub-gradients at point(s) of non-differentiability



■ For a convex, non-diff function f(x), sub-gradient at  $x_*$  is any vector g s.t.  $\forall x$ 

$$f(\mathbf{x}) \ge f(\mathbf{x}_*) + \mathbf{g}^{\mathsf{T}}(\mathbf{x} - \mathbf{x}_*)$$

#### Sub-gradients, Sub-differential, and Some Rules

lacktriangle Set of all sub-gradient at a non-diff point  $oldsymbol{x}_*$  is called the sub-differential

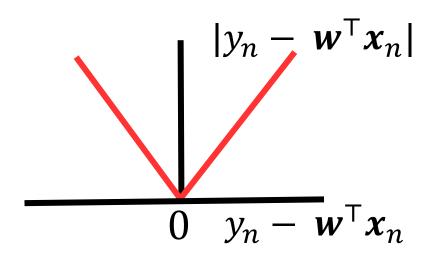
$$\partial f(\mathbf{x}_*) \triangleq \{ \mathbf{g} : f(\mathbf{x}) \geq f(\mathbf{x}_*) + \mathbf{g}^{\mathsf{T}}(\mathbf{x} - \mathbf{x}_*) \ \forall \mathbf{x} \}$$

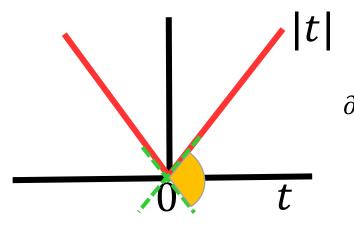
- Some basic rules of sub-diff calculus to keep in mind
  - Scaling rule:  $\partial(c \cdot f(\mathbf{x})) = c \cdot \partial f(\mathbf{x}) = \{c \cdot \mathbf{v} : \mathbf{v} \in \partial f(\mathbf{x})\}$

The affine transform rule is a special case of the more general chain rule

- Sum rule:  $\partial (f(\mathbf{x}) + g(\mathbf{x})) = \partial f(\mathbf{x}) + \partial g(\mathbf{x}) = \{\mathbf{u} + \mathbf{v} : \mathbf{u} \in \partial f(\mathbf{x}), \mathbf{v} \in \partial g(\mathbf{x})\}$
- Affine trans:  $\partial f(\mathbf{a}^\mathsf{T}\mathbf{x} + b) = \mathbf{a} \cdot \partial f(t) = \{\mathbf{a} \cdot c : c \in \partial f(t)\}$ , where  $t = \mathbf{a}^\mathsf{T}\mathbf{x} + b$
- Max rule: If  $h(x) = \max\{f(x), g(x)\}$  then we calculate  $\partial h(x)$  at  $x_*$  as
  - $\blacksquare \text{ If } f(\mathbf{x}_*) > g(\mathbf{x}_*), \partial h(\mathbf{x}_*) = \partial f(\mathbf{x}_*), \text{ If } g(\mathbf{x}_*) > f(\mathbf{x}_*), \partial h(\mathbf{x}_*) = \partial g(\mathbf{x}_*)$
  - If  $f(x_*) = g(x_*)$ ,  $\partial h(x_*) = \{\alpha \mathbf{a} + (1 \alpha)\mathbf{b} : \mathbf{a} \in \partial f(x_*), \mathbf{b} \in \partial g(x_*), \alpha \in [0,1]\}$
- $x_*$  is a stationary point for a non-diff function f(x) if the zero vector belongs to the sub-differential at  $x_*$ , i.e.,  $\mathbf{0} \in \partial f(x_*)$

#### Sub-Gradient For Absolute Loss Regression





Using max rule of subdifferentials and using  $|t| = \max\{t, -t\}$ 

$$\partial |t| = \begin{cases} 1 & \text{if } t > 0 \\ -1 & \text{if } t < 0 \\ [-1, +1] & \text{if } t = 0 \end{cases}$$

- The loss function for linear reg. with absolute loss:  $L(w) = |y_n w^T x_n|$
- Non-differentiable at  $y_n \mathbf{w}^{\mathsf{T}} \mathbf{x}_n = \mathbf{0}$
- Can use the affine transform and max rule of sub-diff calculus
- Assume  $t = y_n \mathbf{w}^{\mathsf{T}} \mathbf{x}_n$ . Then  $\partial L(\mathbf{w}) = -\mathbf{x}_n \partial |t|$ 

  - $\bullet$   $\partial L(\mathbf{w}) = -\mathbf{x}_n \times -1 = \mathbf{x}_n \text{ if } t < 0$
  - $\partial L(\mathbf{w}) = -\mathbf{x}_n \times c = -c\mathbf{x}_n$  where  $c \in [-1, +1]$  if t = 0



#### Sub-Gradient Descent

- Suppose we have a non-differentiable function L(w)
- Sub-gradient descent is almost identical to GD except we use subgradients

#### **Sub-Gradient Descent**

- Initialize  $\boldsymbol{w}$  as  $\boldsymbol{w}^{(0)}$
- For iteration t = 0,1,2,... (or until convergence)
  - lacktriangle Calculate the sub-gradient  $oldsymbol{g}^{(t)} \in \partial L(oldsymbol{w}^{(t)})$
  - Set the learning rate  $\eta_t$
  - Move in the <u>opposite</u> direction of subgradient

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



#### Optimization for ML: Some Final Comments

- Gradient methods are simple to understand and implement
- More sophisticated optimization methods also often use gradient methods
- Backpropagation algo used in deep neural nets is GD + chain rule of differentiation
- Use subgradient methods if function not differentiable
- Constrained optimization can use Lagrangian or projected GD
- Second order methods such as Newton's method faster but computationally expensive
- But computing all this gradient related stuff by hand looks scary to me. Any help?
  - Don't worry. Automatic Differentiation (AD) methods available now (will see them later)
  - AD only requires specifying the loss function (especially useful for deep neural nets)
  - Many packages such as Tensorflow, PyTorch, etc. provide AD support
  - But having a good understanding of optimization is still helpful

