Proposal Due 1/13 11:59 PM

Neural Network Optimization

Machine Learning Problems

- **Given data:**

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- **Learning a model's parameters:** $\min_w \sum_{i=1}^n \ell_i(w)$

w: parameter

$$\text{Logistic Loss: } \ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$$

$$\text{Squared error Loss: } \ell_i(w) = (y_i - x_i^T w)^2$$

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$$\text{Squared error Loss: } \ell_i(w) = (y_i - x_i^T w)^2$$

step size / learning rate

Gradient Descent:

$$w_{t+1} = w_t - \eta \nabla_w \left(\frac{1}{n} \sum_{i=1}^n \ell_i(w) \right) \Big|_{w=w_t}$$

0 initialization for w_0

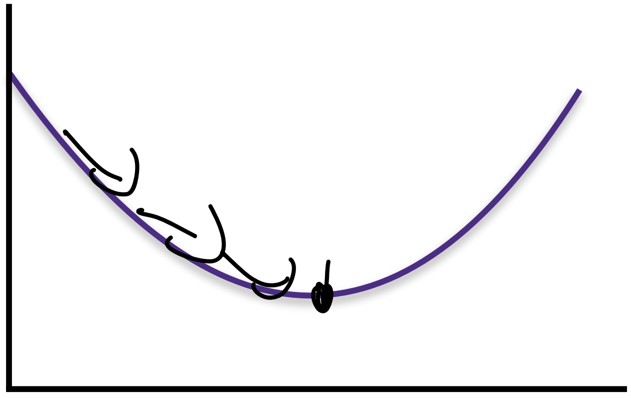
or random init $w_0 \sim D_w$

Gradient Descent

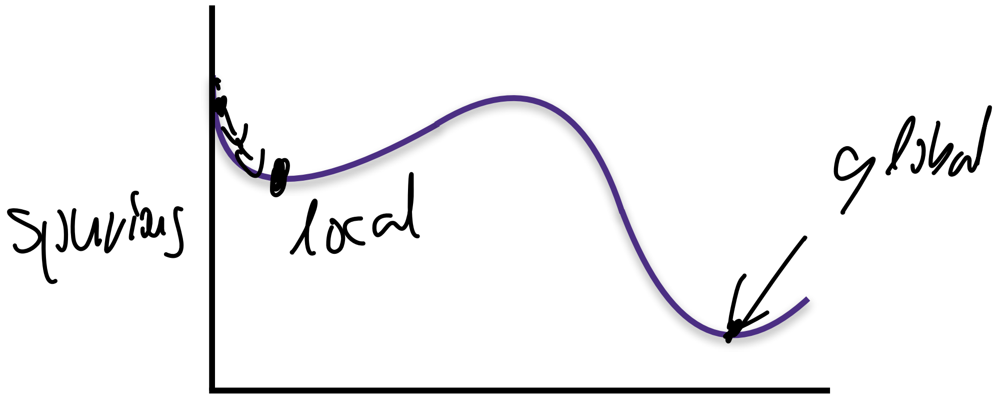
min $f(w)$

$$\text{Initialize: } \underline{w_0 = 0}$$
$$\text{for } t = 1, 2, \ldots$$
$$w_{t+1} = w_t - \eta \nabla f(w_t)$$

Convex Function



Non-convex Function



Sub-Gradient Descent

f is not differentiable

ReLU

Initialize: $w_0 = 0$

for $t = 1, 2, \ldots$

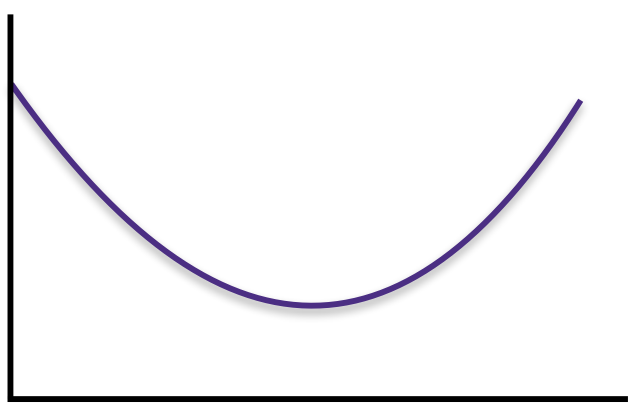
Find any g_t such that $f(y) \geq f(w_t) + g_t^\top (y - w_t)$

$w_{t+1} = w_t - \eta g_t$

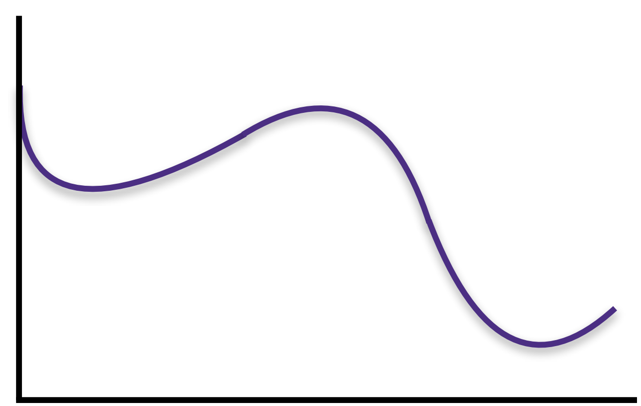
X for NN

g is a subgradient at x if $f(y) \geq f(x) + g^T(y - x)$

Convex Function



Non-convex Function



Machine Learning Problems

- **Given data:**

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- **Learning a model's parameters:** $\sum_{i=1}^n \ell_i(w)$

time complexity

$O(n)$

Gradient Descent:

$$w_{t+1} = w_t - \eta \nabla_w \left(\frac{1}{n} \sum_{i=1}^n \ell_i(w) \right) \Big|_{w=w_t}$$

other distribution

Stochastic Gradient Descent:

$$w_{t+1} = w_t - \eta \nabla_w \ell_{I_t}(w) \Big|_{w=w_t}$$

I_t drawn uniform at random from $\{1, \ldots, n\}$

strongly convex; GD: $\log(\frac{1}{\varepsilon})$

SGD : $\frac{1}{\varepsilon^2}$

$$\mathbb{E}[\nabla_w \ell_{I_t}(w)] = \nabla_w \left(\frac{1}{n} \sum_{i=1}^n \ell_i(w) \right)$$

Mini-batch SGD

Instead of one iterate, average B stochastic gradient together

$$\frac{1}{B}\sum_{i=1}^{B} \nabla_w \ell_{(i)}(w)\Big|_{w=w_t}$$

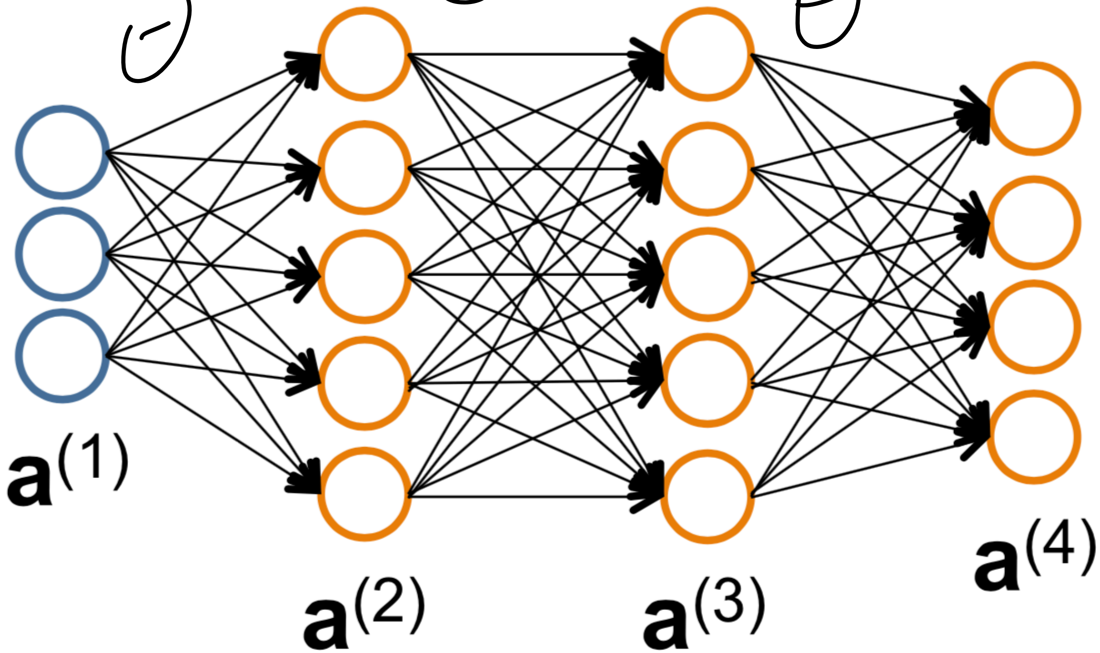
Advantages:

- de-noises gradient
- Matrix computations
- Parallelization

Gradient Computation on a Graph

L : # of layers

$\Theta^{(1)}$ $\Theta^{(2)}$ $\Theta^{(2)}$



Naive computation: node by node

$$\frac{\partial L}{\partial \Theta^{(1)}} : O(L), \Rightarrow O(L^2)$$

A brief history

- **Back propagation:** the workhorse for training neural networks. An algorithm that for a network with V nodes and E edges calculates that gradient in **linear time** O(V+E).
- The name was introduced by Rumelhart, Hinton, Williams '86. Same idea was rediscovered multiple times. Also mentioned in Werbos' thesis '74 in the context of neural networks.
- **Control theory:** Kelly '60, Bryson '61 [**dynamic programming**]
- **Theoretical computer science:** Baur-Strassen lemma '83 [**algebraic circuits**]

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

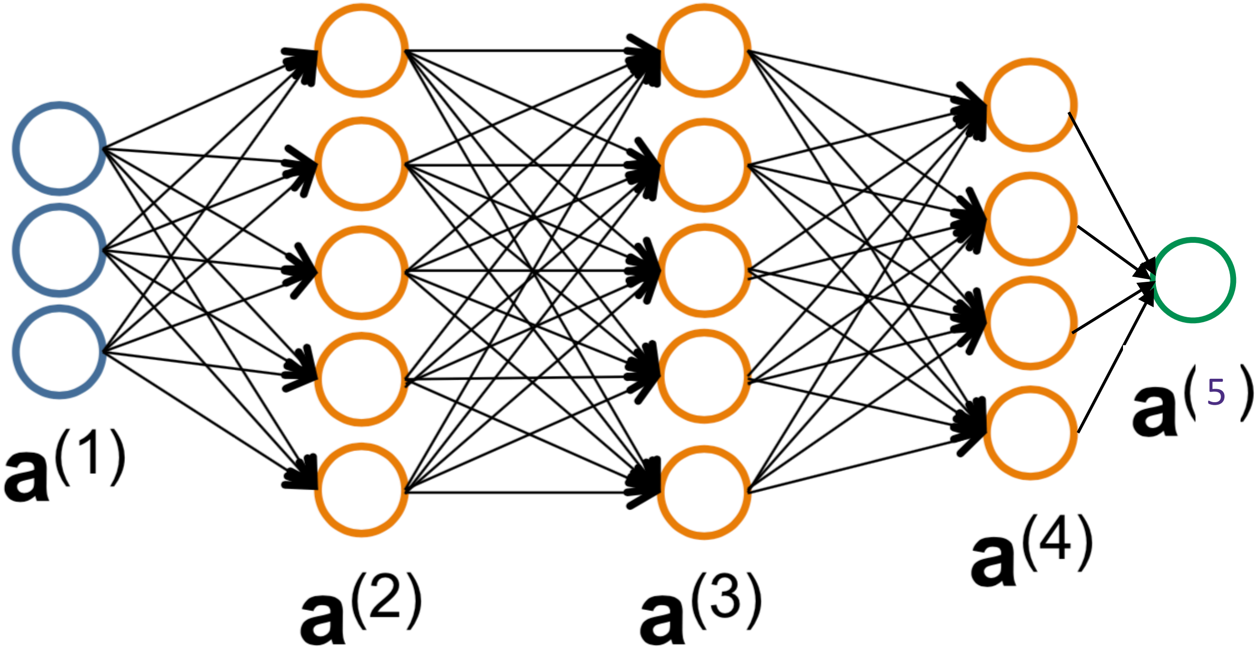
$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = g(\Theta^{(L)} a^{(L)})$$



$$L(y, \hat{y}) = y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}}$$

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \underbrace{\nabla_{\Theta^{(l)}} L(y, \hat{y})}$ $\forall l$

Goal

Forward Propagation

L: # of layers
Ignore bias
g: activation func
$z^{(l)}$: pre-activation

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

⋮

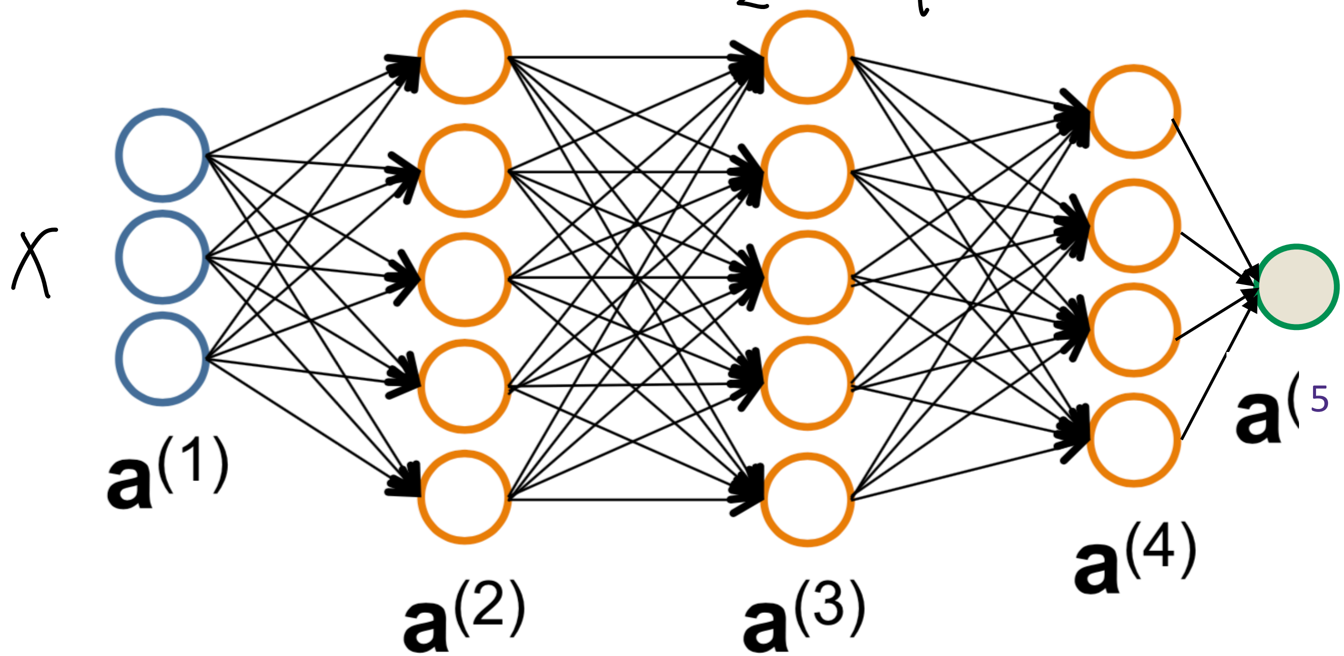
$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

⋮

$$\hat{y} = a^{(L+1)}$$



$$L(y, \hat{y}) = y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}}$$

Backprop

$x \in \mathbb{R}^d$, $\Theta^{(1)}, \ldots, \Theta^{(L)}$ parameters to train

$\Theta^{(1)} \in \mathbb{R}^{m \times d}$, $\Theta^{(2)} \ldots \Theta^{(L-1)} : \mathbb{R}^{m \times m}$, $\Theta^{(L)} : \mathbb{R}^{m}$

m: width

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = a^{(L+1)}$$

Train by Stochastic Gradient Descent:

scalar

$$\Theta^{(l)}_{i,j} \leftarrow \Theta^{(l)}_{i,j} - \eta \frac{\partial L(y, \widehat{y})}{\partial \Theta^{(l)}_{i,j}}$$

wrt for all i, j, l

$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1 - y)\log(1 - \widehat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}}$$

Chain Rule $z_i^{(l+1)} = \sum_{j=1}^{m} \theta_{ij}^{(l)} \cdot a_j^{(l)}$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

Train by Stochastic Gradient Descent:

$$\Theta_{i,j}^{(l)} \leftarrow \Theta_{i,j}^{(l)} - \eta \frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}}$$

$$L(y, \hat{y}) = y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = a^{(L+1)}$$

$$\boxed{\frac{\partial L(y,\widehat{y})}{\partial \Theta^{(l)}_{i,j}} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta^{(l)}_{i,j}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}}$$

chain Rule

$$\delta_i^{(l)} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l)}} = \sum_k \overbrace{\frac{\partial L(y,\widehat{y})}{\partial z_k^{(l+1)}}}^{\delta_k^{(l+1)}} \cdot \underbrace{\frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}}}_{\Theta_{ki}^{(l)} \cdot g'(z_i^{(l)})}$$

$$z_k^{(l+1)} = \sum_{u=1}^{m} \Theta_{ku}^{(l)} \cdot g(z_u^{(l)})$$

$$L(y,\widehat{y}) = y\log(\widehat{y}) + (1-y)\log(1-\widehat{y})$$

$$g(z) = \frac{1}{1+e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

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$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

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$$\widehat{y} = a^{(L+1)}$$

$$\boxed{\frac{\partial L(y,\widehat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}}$$

$$\delta_i^{(l)} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l)}} = \sum_k \frac{\partial L(y,\widehat{y})}{\partial z_k^{(l+1)}} \cdot \frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}}$$

$$= \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)} \, g'(z_i^{(l)})$$

$$= \underline{a_i^{(l)}(1 - a_i^{(l)})} \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

$$L(y,\widehat{y}) = y \log(\widehat{y}) + (1-y)\log(1-\widehat{y})$$

$$g(z) = \frac{1}{1+e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}}$$

Backprop

Recursion / Dynamic Programming

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

$$\begin{array}{cccc} \delta^{(l+1)} \to & \delta^{(l)} \to & \cdots \to & \delta^{(1)} \\ & \downarrow & & \downarrow \\ & \Theta^{(l)} \to & \cdots \to & \Theta^{(1)} \end{array}$$

$$L(y, \hat{y}) = y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \widehat{y})}{\partial \Theta^{(l)}_{i,j}} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta^{(l)}_{i,j}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta^{(l)}_{k,i}$$

$$\delta_i^{(L+1)} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(L+1)}} = \frac{\partial}{\partial z_i^{(L+1)}} \left[y \log(g(z^{(L+1)})) + (1-y)\log(1 - g(z^{(L+1)})) \right]$$

$$= \frac{y}{g(z^{(L+1)})} g'(z^{(L+1)}) - \frac{1-y}{1 - g(z^{(L+1)})} g'(z^{(L+1)})$$

$$= y - g(z^{(L+1)}) = y - a^{(L+1)}$$

$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1-y)\log(1 - \widehat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}}$$

Backprop

Time : $O(L)$

$$a^{(1)} = x$$

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$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

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$$\widehat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \widehat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

$$\delta^{(L+1)} = y - a^{(L+1)}$$

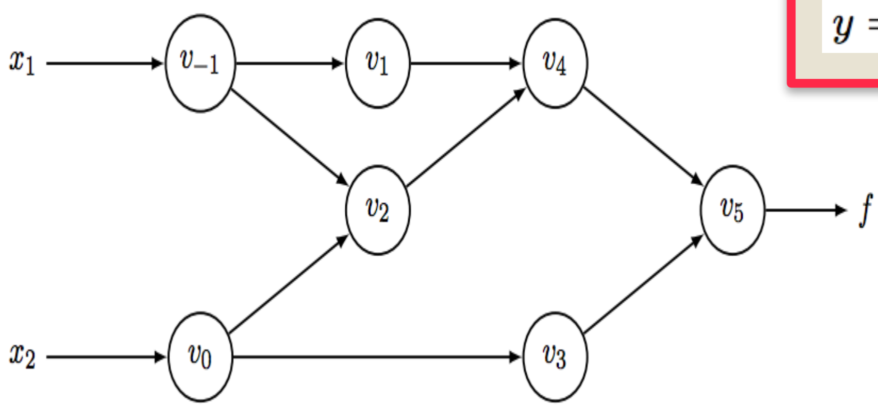
Recursive Algorithm!

$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1 - y)\log(1 - \widehat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}}$$

Auto-differentiation

Backprop for this simple network architecture is a special case of ***reverse-mode auto-differentiation:***



$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$

Forward Primal Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint (Derivative) Trace			
$\bar{\boldsymbol{x}}_1$	$= \bar{\boldsymbol{v}}_{-1}$		$= \mathbf{5.5}$
$\bar{\boldsymbol{x}}_2$	$= \bar{\boldsymbol{v}}_0$		$= \mathbf{1.716}$
$\bar{v}_{-1}$	$= \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0$	$= \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Auto-differentiation

- Given a function, computes its partial derivatives
- Compute all of the partial derivatives of a function with (nearly) same computation runtime [Griewank '89, Baur and Strassen '83]

  of computing the function
- Backbone of (applied) machine learning: Pytorch, Tensorflow, …

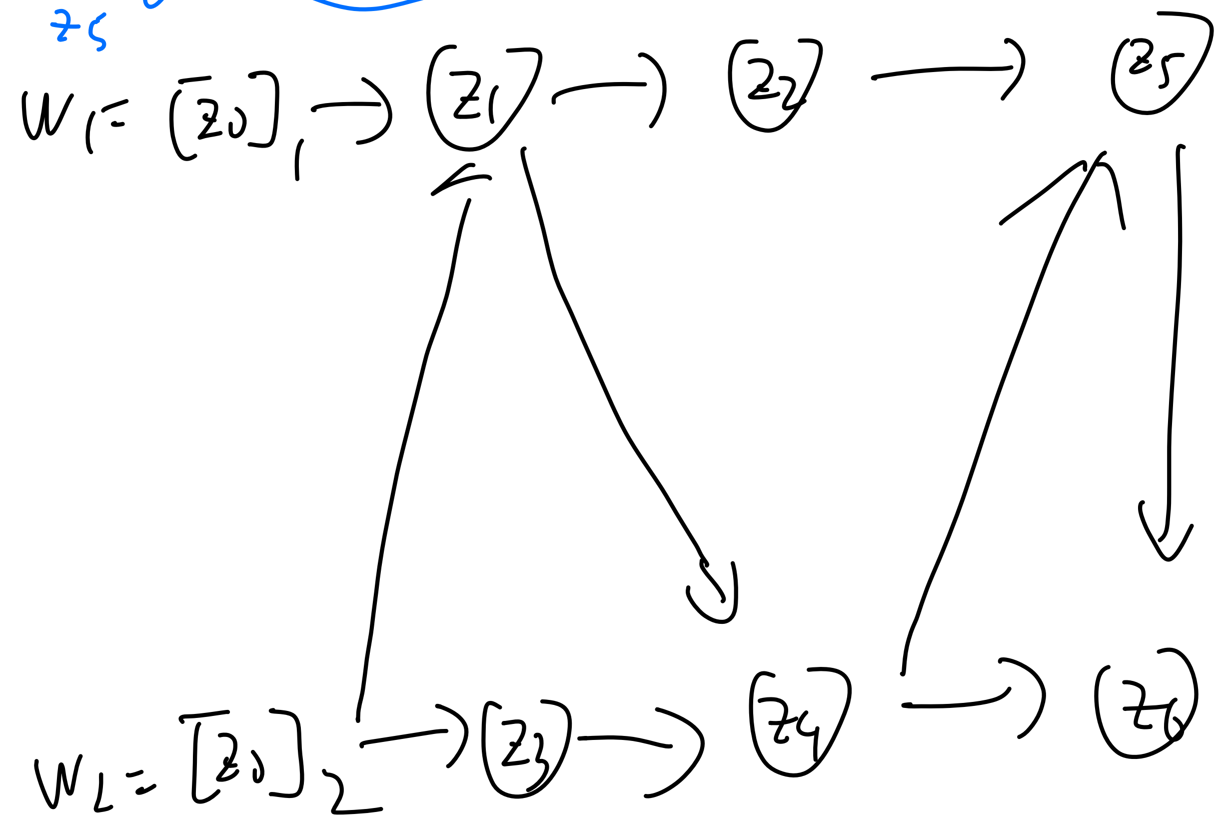
Example of Computation Graph

$$f(w_1, w_2) = \underbrace{\left(\overbrace{\sin\left(\frac{2\pi w_1}{w_2}\right)}^{z_2} + \frac{3\overbrace{w_1}^{z_1}}{w_2} - \overbrace{\exp(2w_2)}^{z_3} \right)}_{z_5} \cdot \overbrace{\left(\frac{3w_1}{w_2} - \exp(2w_2) \right)}^{z_4}$$

Input: $z_0 = (w_1, w_2)$

1. $z_1 = \frac{w_1}{w_2}$
2. $z_2 = \sin(2\pi \cdot z_1)$
3. $z_3 = \exp(2w_2)$
4. $z_4 = 3z_1 - z_3$
5. $z_5 = z_2 + z_4$
6. $z_6 = z_4 \cdot z_5$

return z_6



Computation Model

- Given access to a set of differentiable real functions $h \in \mathscr{H}$
- Use functions in $\mathscr{H}$ to create intermediate variables.
- Evaluation trace:
  - All intermediate variables will be scalars; each corresponds to a node.
  - Input $z_0 = w \in \mathbb{R}^d$. $[z_0]_1 = w_1, [z_0]_2 = w_2, \ldots, [z_0]_d = w_d$
  - Step 1: $z_1 = h_1$ (a subset of variables in w)
  - …. $z_2 = h_2(z_1, w)$
  - Step t: $z_t = h_t$ (a subset of variables in $z_1, \ldots, z_{t-1}, w$)
  - …
  - Step T: $z_T = h_T$ (a subset of variables in $z_1, \ldots, z_{T-1}, w$)
  - **Return:** z_T

($h_1, \ldots, h_T \in \mathscr{H}$)

Computation Model

NN

- Every $h \in \mathscr{H}$ is one of the following:
  - Type 1: An affine transformation of the inputs

    $3z_1 - z_3, \quad z_2 + z_5, \quad z_1 + z_2 + 6$

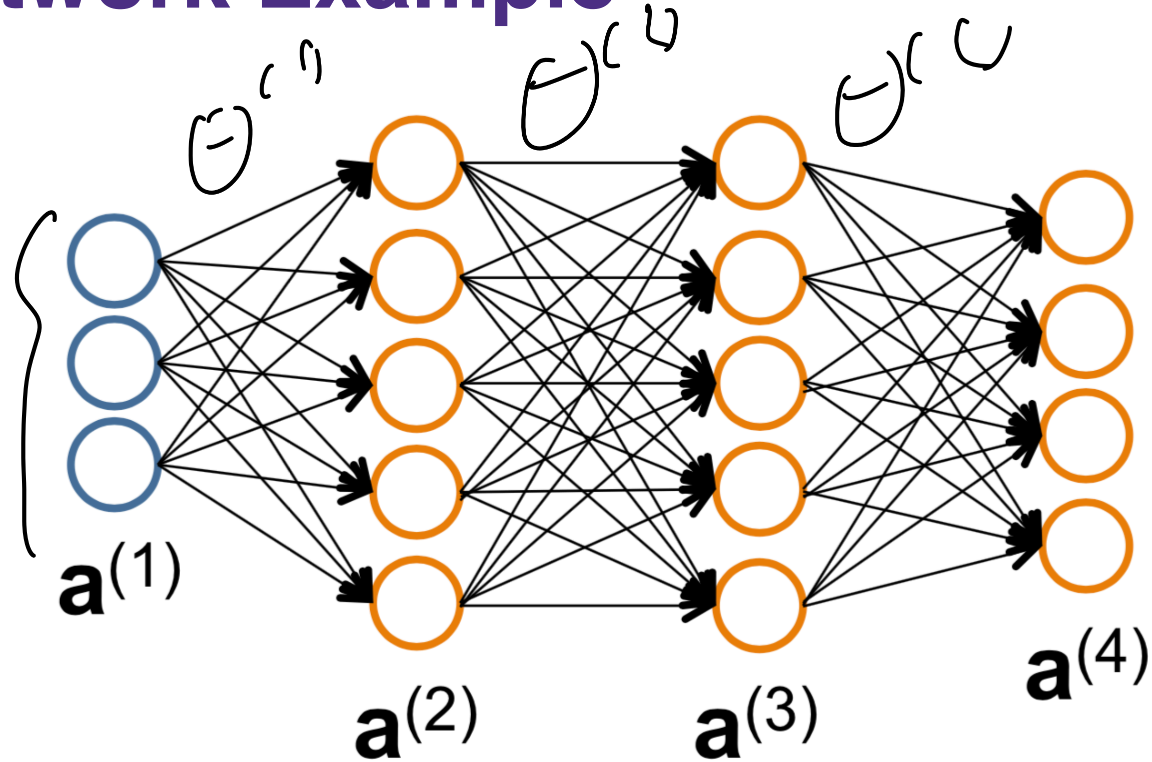
  - Type 2: A product of variables, to some power

    $w_1 / w_2, \quad z_3 \cdot z_4, \quad z_7 = z_1^4 \, z_5^7 \, z_6^{-1}$

  - Type 3: A fixed set of one dimensional differentiable functions: $\sin(\cdot), \cos(\cdot), \exp(\cdot), \log(\cdot), \ldots$
    - We assume we can easily compute the derivatives for each of this functions. $O(1)$
    - Type 3 can be approximated by Type 1 and Type 2, using polynomials.

Neural Network Example

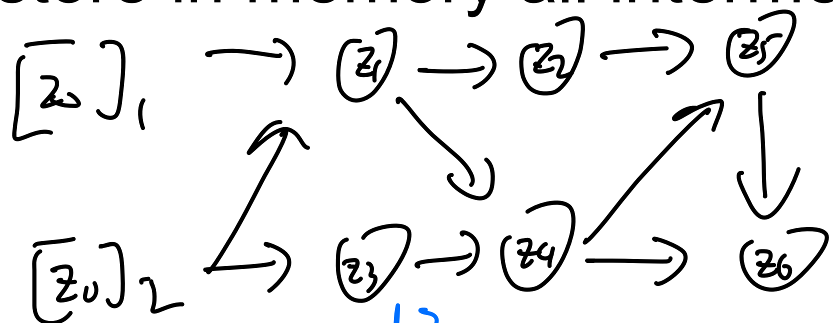
Constant



Reverse Mode of Automatic Differentiation

Goal: Compute partial derivatives of $f(w)$, i.e., df/dw.

- Step 1: computer $f(w)$ and store in memory all intermediate variables $z_1, \ldots, z_T$ forward pass



- Step 2: Initialize: $\dfrac{dz_T}{dz_T} = 1.$
- Step 3: For $t = T, T-1, \ldots, 0$
  - $$\frac{dz_T}{dz_t} \overset{\text{Chain rule}}{=} \sum_{c \text{ is a child of } t} \frac{dz_T}{dz_c} \cdot \frac{\partial z_c}{\partial z_t}$$

(Child: a node z_t directly points to)

- Step 4: Return $\dfrac{dz_T}{dz_0} = \dfrac{df}{dw}$

(1) $\dfrac{dz_6}{dz_6} = 1$

(2) $\dfrac{dz_6}{dz_5} = \dfrac{dz_6}{dz_6} \cdot \dfrac{\partial z_6}{\partial z_5}$

(3) $\dfrac{dz_6}{dz_4} = \dfrac{dz_6}{dz_5} \cdot \dfrac{\partial z_5}{\partial z_4} + \dfrac{dz_6}{dz_6} \cdot \dfrac{\partial z_6}{\partial z_4}$

(4) $\dfrac{dz_6}{dz_3} = \dfrac{dz_6}{dz_4} \cdot \dfrac{\partial z_4}{\partial z_3}$

(5) $\dfrac{dz_6}{dz_2} = \dfrac{dz_6}{dz_5} \cdot \dfrac{\partial z_5}{\partial z_2}$

(6) $\dfrac{dz_6}{dz_1} = \dfrac{dz_6}{dz_2} \cdot \dfrac{\partial z_2}{\partial z_1} + \dfrac{dz_6}{dz_4} \cdot \dfrac{\partial z_4}{\partial z_1}$

Time Complexity

Theorem (Baur and Strassen '83, Griewak '89): Assume every h is specified as in our computational model. For $h(\cdot)$ of type 3, assume we can compute the derivative $h'(z)$ in time as the same order of computing $h(z)$. Let T denote the time to compute $f(w)$. Then the reverse mode computes df/dw in time $O(T)$.

pf: ① correctness: $\frac{dz_T}{dz_c}$ is already computed

to compute $\frac{dz_T}{dz_t}$, need $\frac{\partial z_c}{\partial z_t}$ can be computed

type 1: $z_c = a^T (z_1, \cdots, z_t) + b \rightarrow$ coefficient

type 2: product: $\frac{\partial z_c}{\partial z_t} = \alpha \cdot \frac{z_c}{z_t}$, α: exponent, $z_c = z_1 \cdot z_t^2$

type 3: $z_c = h(z_t)$, $\Rightarrow \frac{\partial z_c}{\partial z_t} = h'(z_t)$

② Time: $O(V+E)$

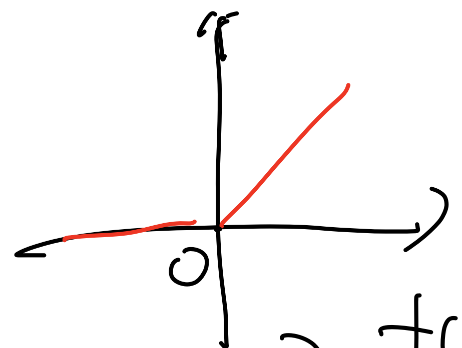
Clarke Differential

Subdifferential and Subgradient

Definition: Given $f : \mathbb{R}^d \to \mathbb{R}$, for every x, the subdifferential set is defined as $\partial_s f(x) \triangleq \{s \in \mathbb{R}^d : \forall x' \in \mathbb{R}^d, f(x') \geq f(x) + s^\top (x' - x)\}$. The elements in the subdifferential set are subgradients.

$g_t \in \partial_s f(x)$

$x_{t+1} \leftarrow x_t - \eta g_t$



$\partial_0 f(0) = [0, 1]$

Subdifferential and Subgradient

Definition: Given $f : \mathbb{R}^d \to \mathbb{R}$, for every x, the subdifferential set is defined as
$\partial_s f(x) \triangleq \{s \in \mathbb{R}^d : \forall x' \in \mathbb{R}^d, f(x') \geq f(x) + s^\top (x' - x)\}$. The elements in the subdifferential set are subgradients.

- If f is convex $\to$ $\partial_s f$ exists everywhere
- If f is convex & differentiable

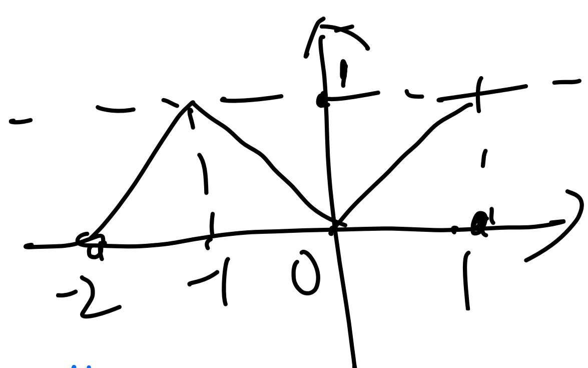
$$\partial_s f = \{\nabla f\}$$

- $O\left(\frac{1}{\sqrt{T}}\right)$ rate

Subdifferential is not enough

Definition: Given $f : \mathbb{R}^d \to \mathbb{R}$, for every x, the subdifferential set is defined as $\partial_s f(x) \triangleq \{s \in \mathbb{R}^d : \forall x' \in \mathbb{R}^d, f(x') \geq f(x) + s^\top(x' - x)\}$. The elements in the subdifferential set are subgradients.

Problem: NN is not convex



$x = -1$

we need s s.t. $\forall x'$

$f(x') \geq 1 + s \cdot (x' - (-1))$

- choose $x' = -2$

$0 \geq 1 + s \cdot (-2 - (-1))$

$\Rightarrow s \geq 1$

- choose $x' = 1$

$1 \geq 1 + s \cdot 2 \Rightarrow s \leq 0$

subgradient is not well-defined

Clarke Differential

Pick $g_t \in \partial f(x)$

$x_{t+1} \leftarrow x_t - \eta g_t$

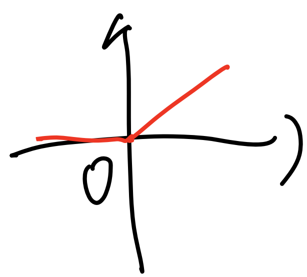
Definition: Given $f : \mathbb{R}^d \to \mathbb{R}$, for every x, the Clark differential is defined as

$$\partial f(x) \triangleq \text{conv}\left(\{s \in \mathbb{R}^d : \exists \{x_i\}_{i=1}^{\infty} \to x, \{\nabla f(x_i)\}_{i=1}^{\infty} \to s\}\right).$$

The elements in the subdifferential set are subgradients.

$\text{conv}(S) = \{v : v = \sum_{i=1}^{n} \lambda_i u_i,\ u_i \in S,\ \lambda_i \geq 0,\ \sum_{i=1}^{n} \lambda_i = 1\}$

ReLU :

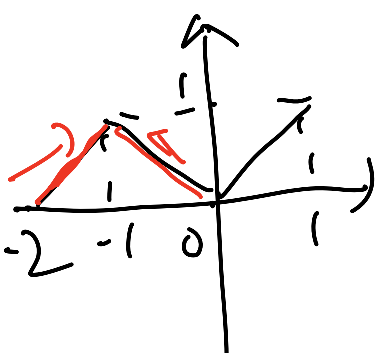


$\{x_i\}$, $-1, -\frac{1}{2}, \dots \to 0$

$\nabla f(x_i) = 0$

$\{x_i\}$, $1, \frac{1}{2}, \dots \to 0$

$\nabla f(x_i) = 1 \to 1$, $\partial f(0) = [0,1]$



$\partial f(-1)$

$\{x_i\} : -2, -1.5, \dots \to -1$, $\nabla f(x_i) = 1$

$\{x_i\} : 0, -\frac{1}{2}, \dots \to -1$, $\nabla f(x_i) = -1$, $\partial f(x) = [-1, 1]$

When does Clarke differential exists

Definition (Locally Lipschitz): $f : \mathbb{R}^d \to \mathbb{R}$ is locally Lipchitz if $\forall x \in \mathbb{R}^d$, there exists a neighborhood S of x, such that f is Lipchitz in S.

$\forall x, x' \in S \quad |f(x) - f(x')| \leq L \cdot \|x - x'\|$

- If locally Lip $\Rightarrow \partial f$ exists everywhere
- If f is convex $\rightarrow \partial f = \partial_s f$
- If f is differentiable $\Rightarrow \partial f(x) = \{\nabla f(x)\}$

✡ satisfies chain rule