# 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:** $\displaystyle\sum_{i=1}^n \ell_i(w)$

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

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

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Gradient Descent:

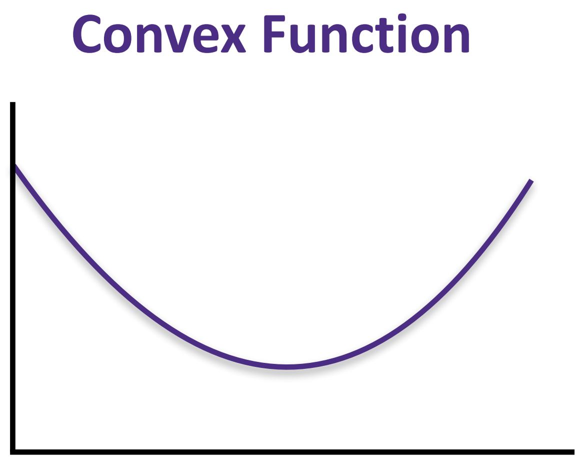
$$w_{t+1} = w_t - \eta \nabla_w \left( \frac{1}{n} \sum_{i=1}^n \ell_i(w) \right) \Big|_{w=w_t}$$

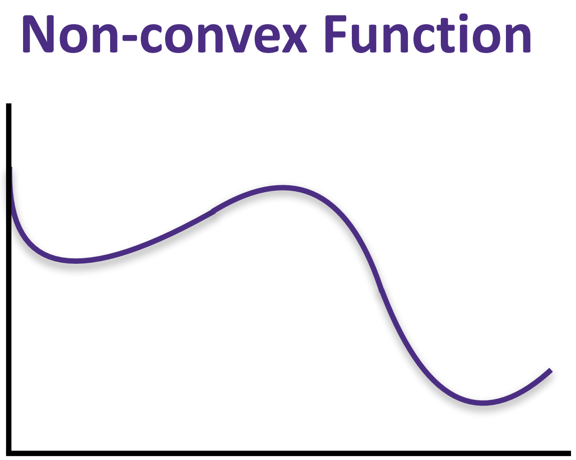
# Gradient Descent

Initialize: $w_0 = 0$

for $t = 1, 2, \ldots$

$$w_{t+1} = w_t - \eta \nabla f(w_t)$$



# Sub-Gradient Descent

Initialize: $w_0 = 0$

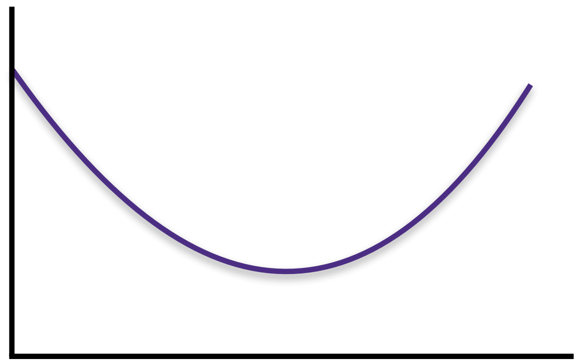
for $t = 1, 2, \ldots$

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

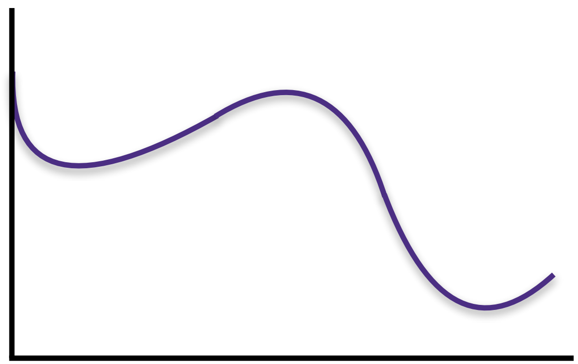
$w_{t+1} = w_t - \eta g_t$

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

Convex Function



Non-convex Function



# Machine Learning Problems

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

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

Gradient Descent:

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

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 $\{1, \ldots, n\}$

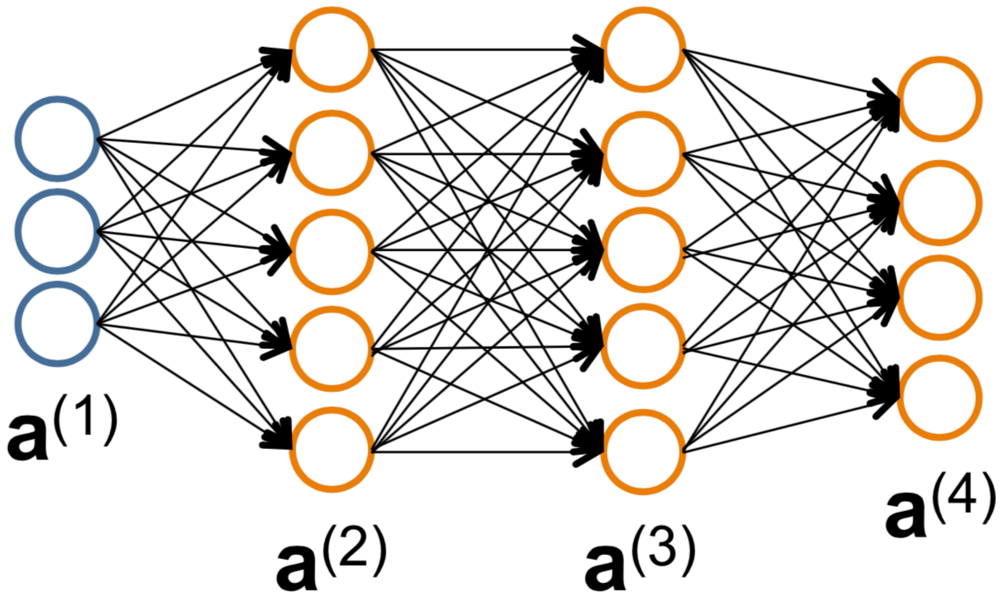
# Mini-batch SGD

Instead of one iterate, average B stochastic gradient together

Advantages:

- de-noises gradient
- Matrix computations
- Parallelization

# Gradient Computation on a Graph




Naive computation: node by node

# 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**]

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

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

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

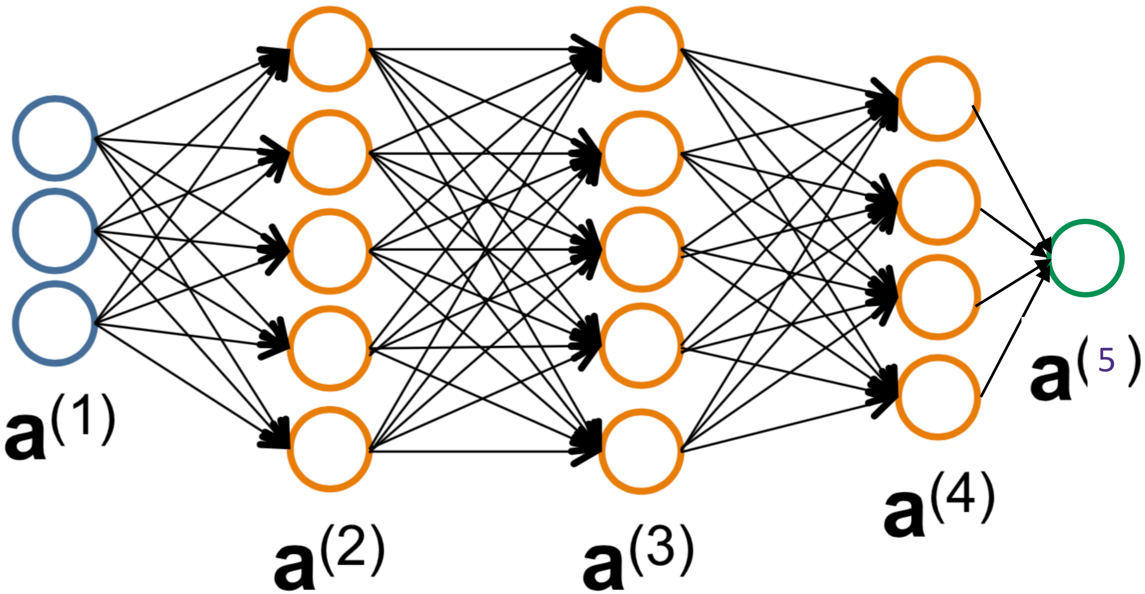
$$\vdots$$

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

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

$$\vdots$$

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




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

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

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

# Forward Propagation

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

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

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

$$\vdots$$

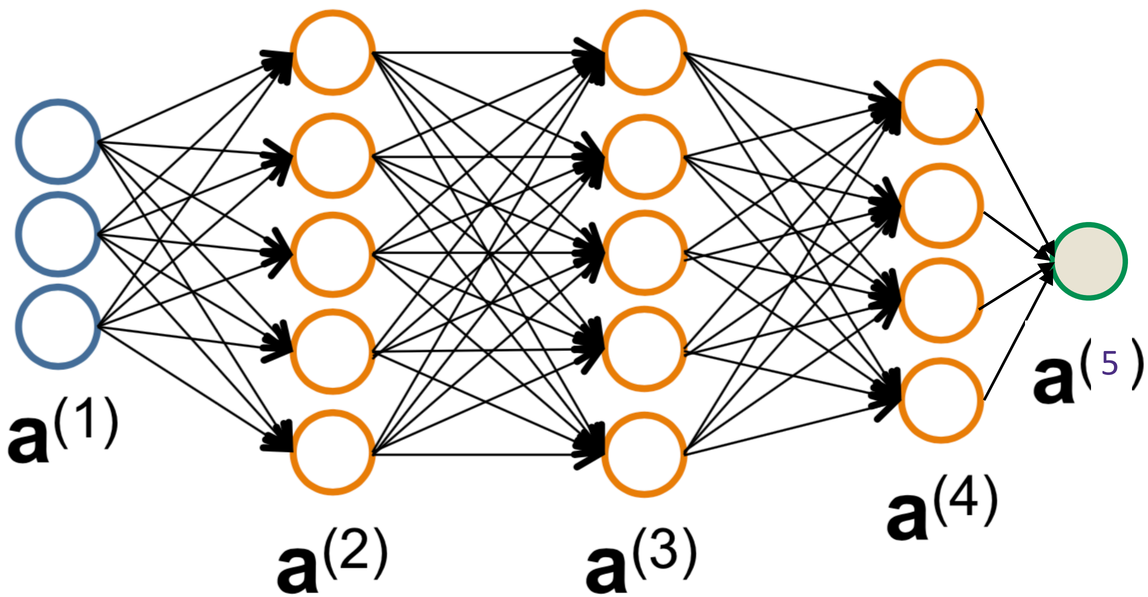
$$a^{(l)} = g(z^{(l)})$$

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

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

$$\vdots$$

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




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

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

# Backprop

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

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

$$\vdots$$

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

**Train by Stochastic Gradient Descent:**

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

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

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

# Backprop

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

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

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

$\vdots$

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

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

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

$\vdots$

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

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

**Train by Stochastic Gradient Descent:**

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

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

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

# Backprop

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

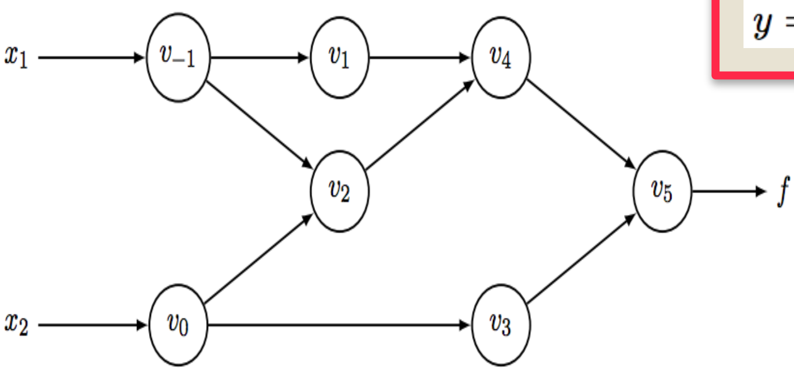
Recursive Algorithm!

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

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

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

# 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]
- Backbone of (applied) machine learning: Pytorch, Tensorflow, …

# Example of Computation Graph

$$f(w_1, w_2) = \left( \sin\left(\frac{2\pi w_1}{w_2}\right) + \frac{3w_1}{w_2} - \exp(2w_2) \right) \cdot \left( \frac{3w_1}{w_2} - \exp(2w_2) \right)$$

**Input**: $z_0 = (w_1, w_2)$

# Computation Model

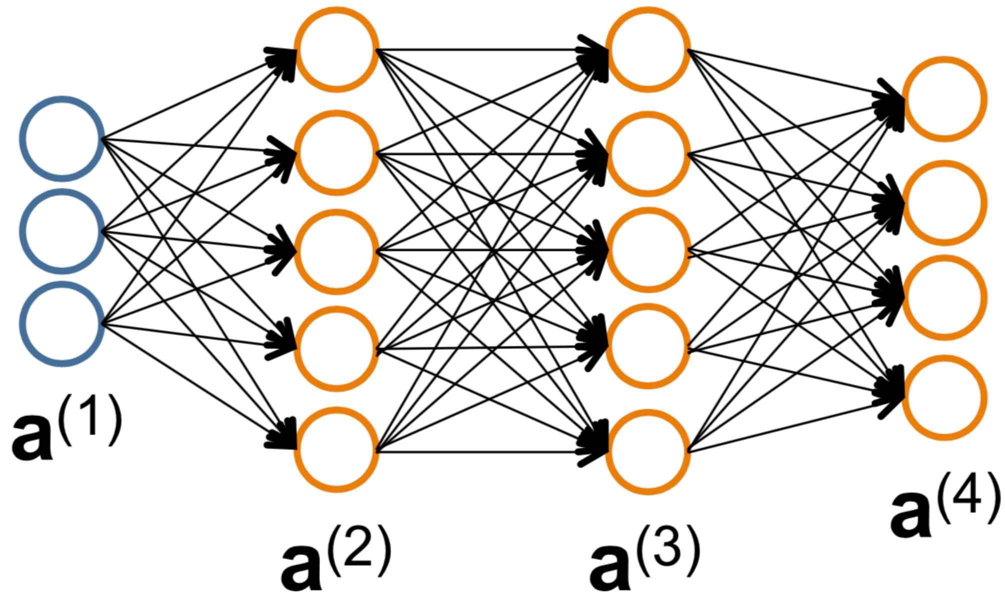
- Given access to a set of differentiable real functions $h \in \mathscr{H}$
- Use functions in $\mathscr{H}$ to create intermediate variables.
- Evaluation trace:
  - All intermediate variables will be scalars; each corresponds to a node.
  - Input $z_0 = w \in \mathbb{R}^d$. $[z_0]_1 = w_1, [z_0]_2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

- Every $h \in \mathscr{H}$ is one of the following:
  - Type 1: An affine transformation of the inputs
  - Type 2: A product of variables, to some power
  - 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.
    - Type 3 can be approximated by Type 1 and Type 2, using polynomials.

# Neural Network Example



# 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 $z_1, \ldots, z_T$
- Step 2: Initialize: $\dfrac{dz_T}{dz_T} = 1.$
- Step 3: For $t = T, T-1, \ldots, 0$
  - $$\frac{dz_T}{dz_t} = \sum_{\text{c is a child of t}} \frac{dz_T}{dz_c} \cdot \frac{\partial z_c}{\partial z_t}$$

  (Child: a node $z_t$ directly points to)
- Step 4: Return $\dfrac{dz_T}{dz_0} = \dfrac{df}{dw}$

# 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 $O(T)$.

# Time Complexity

# 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.

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# 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.

# Clarke Differential

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

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

The elements in the subdifferential set are subgradients.

# 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 $S$.