10-301/10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Backpropagation

Matt Gormley
Lecture 13
Oct. 9, 2023

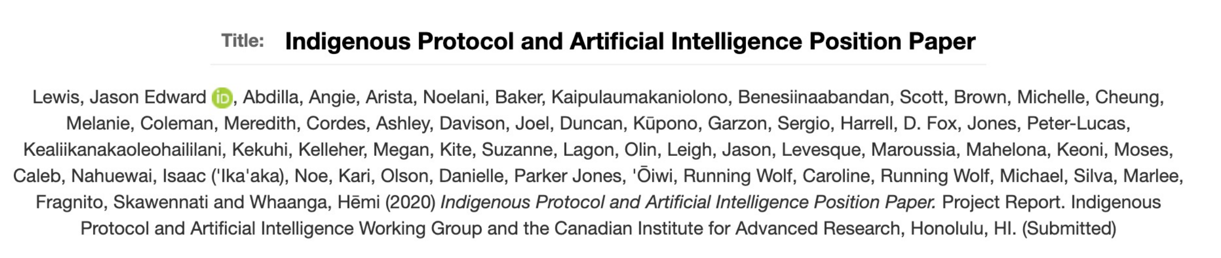
Reminders

- Homework 4: Logistic Regression
  - Out: Fri, Sep 29
  - Due: Mon, Oct 9 at 11:59pm
- Homework 5: Neural Networks
  - Out: Mon, Oct 9
  - Due: Fri, Oct 27 at 11:59pm

Q&A

Q: Happy Indigenous Peoples Day! What do indigenous people have to say about AI and Machine Learning?

A: I’d recommend reading a position paper about that very topic:



Title: **Indigenous Protocol and Artificial Intelligence Position Paper**

Lewis, Jason Edward, Abdilla, Angie, Arista, Noelani, Baker, Kaipulaumakaniolono, Benesiinaabandan, Scott, Brown, Michelle, Cheung, Melanie, Coleman, Meredith, Cordes, Ashley, Davison, Joel, Duncan, Kūpono, Garzon, Sergio, Harrell, D. Fox, Jones, Peter-Lucas, Kealiikanakaoleohaililani, Kekuhi, Kelleher, Megan, Kite, Suzanne, Lagon, Olin, Leigh, Jason, Levesque, Maroussia, Mahelona, Keoni, Moses, Caleb, Nahuewai, Isaac ('Ika'aka), Noe, Kari, Olson, Danielle, Parker Jones, 'Ōiwi, Running Wolf, Caroline, Running Wolf, Michael, Silva, Marlee, Fragnito, Skawennati and Whaanga, Hēmi (2020) *Indigenous Protocol and Artificial Intelligence Position Paper.* Project Report. Indigenous Protocol and Artificial Intelligence Working Group and the Canadian Institute for Advanced Research, Honolulu, HI. (Submitted)

“This position paper on Indigenous Protocol (IP) and Artificial Intelligence (AI) is a starting place for those who want to design and create AI from an ethical position that centers Indigenous concerns. Each Indigenous community will have its own particular approach to the questions we raise in what follows. What we have written here is not a substitute for establishing and maintaining relationships of reciprocal care and support with specific Indigenous communities. Rather, this document offers a range of ideas to take into consideration when entering into conversations which prioritize Indigenous perspectives in the development of artificial intelligence. It captures multiple layers of a discussion that happened over 20 months, across 20 time zones, during two workshops, and between Indigenous people (and a few non-Indigenous folks) from diverse communities in Aotearoa, Australia, North America, and the Pacific.”

https://spectrum.library.concordia.ca/986506/7/Indigenous_Protocol_and_AI_2020.pdf

Algorithm

BACKPROPAGATION FOR A SIMPLE COMPUTATION GRAPH

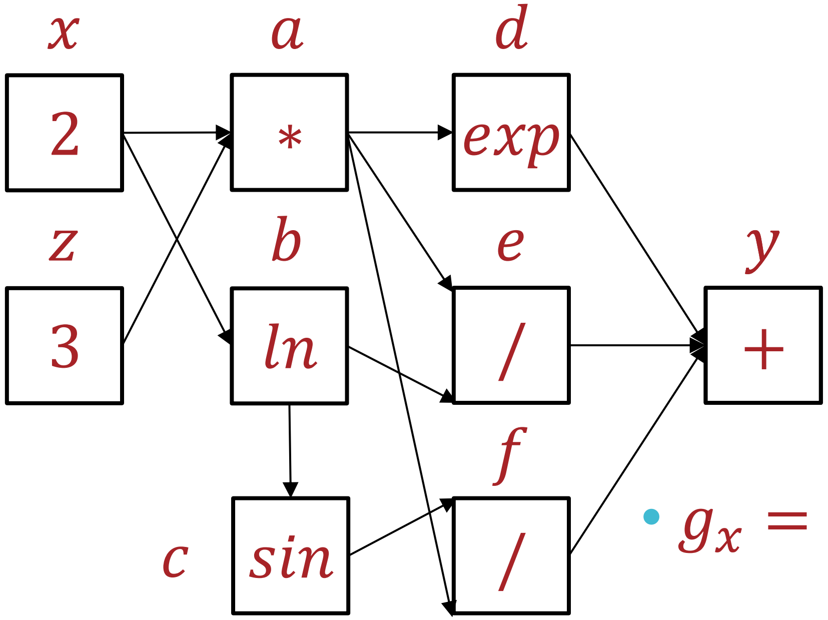
Approach 3: Automatic Differentiation (reverse mode)

- Given

$$y = f(x,z) = e^{xz} + \frac{xz}{\ln(x)} + \frac{\sin(\ln(x))}{xz}$$

what are ${\partial y}/_{\partial x}$ and ${\partial y}/_{\partial z}$ at $x = 2, z = 3$?

- Then compute partial derivatives, starting from y and working back



- $g_y = \frac{\partial y}{\partial y} = 1$
- $g_d = g_e = g_f = 1$
- $g_c = \frac{\partial y}{\partial c} = \frac{\partial y}{\partial f}\frac{\partial f}{\partial c} = g_f\left(\frac{1}{a}\right)$
- $g_b = \frac{\partial y}{\partial b} = \frac{\partial y}{\partial e}\frac{\partial e}{\partial b} + \frac{\partial y}{\partial c}\frac{\partial c}{\partial b}$
  $= g_e\left(-\frac{a}{b^2}\right) + g_c(\cos(b))$
- $g_a = \frac{\partial y}{\partial a} = \frac{\partial y}{\partial f}\frac{\partial f}{\partial a} + \frac{\partial y}{\partial e}\frac{\partial e}{\partial a} + \frac{\partial y}{\partial d}\frac{\partial d}{\partial a}$
  $= g_f\left(\frac{-c}{a^2}\right) + g_e\left(\frac{1}{b}\right) + g_d(e^a)$
- $g_x = \frac{\partial y}{\partial x} = \frac{\partial y}{\partial b}\frac{\partial b}{\partial x} + \frac{\partial y}{\partial a}\frac{\partial a}{\partial x} = g_b\left(\frac{1}{x}\right) + g_a(z)$
- $g_z = \frac{\partial y}{\partial z} = \frac{\partial y}{\partial a}\frac{\partial a}{\partial z} = g_a(x)$

Given

$$y = f(x,z) = e^{xz} + \frac{xz}{\ln(x)} + \frac{\sin(\ln(x))}{xz}$$

t are ${\partial y}/{\partial x}$ and ${\partial y}/{\partial z}$ at $x = 2, z = 3$?

en compute partial derivatives,

rting from y and working back

Approach 2:

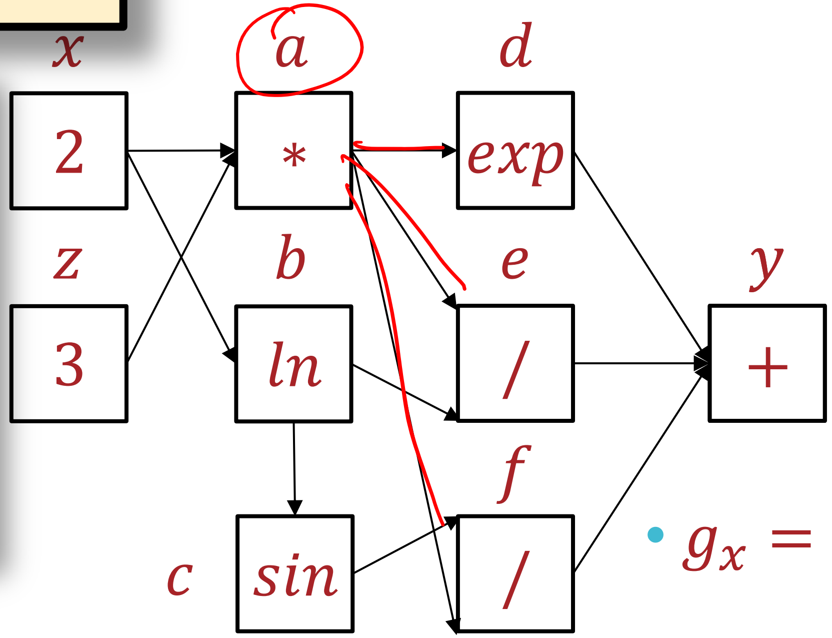
Updates for Backpropagation:

output

$$\underline{g_x} = \frac{\partial \boxed{y}}{\partial x} = \sum_{k=1}^{K} \underbrace{\frac{\partial y}{\partial u_k}} \frac{\partial u_k}{\partial x}$$

$$= \sum_{k=1}^{K} g_{u_k} \frac{\partial u_k}{\partial x}$$

Backprop is efficient b/c of reuse in the forward pass and the backward pass.

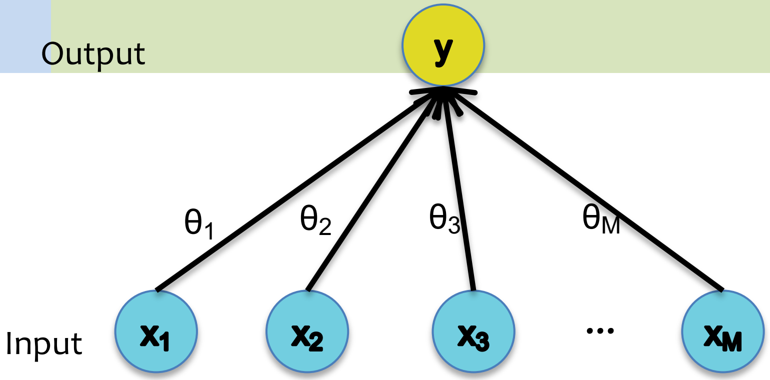


- $g_y = \frac{\partial y}{\partial y} = 1$
- $g_d = g_e = g_f = 1$
- $g_c = \frac{\partial y}{\partial c} = \boxed{\frac{\partial y}{\partial f}} \frac{\partial f}{\partial c} = \boxed{g_f}\left(\frac{1}{a}\right)$
- $g_b = \frac{\partial y}{\partial b} = \frac{\partial y}{\partial e}\frac{\partial e}{\partial b} + \frac{\partial y}{\partial c}\frac{\partial c}{\partial b}$
  $= g_e\left(-\frac{\boxed{a}}{b^2}\right) + g_c(\cos(b))$
- $g_a = \frac{\partial y}{\partial a} = \boxed{\frac{\partial y}{\partial f}}\frac{\partial f}{\partial a} + \frac{\partial y}{\partial e}\frac{\partial e}{\partial a} + \frac{\partial y}{\partial d}\frac{\partial d}{\partial a}$
  $= \boxed{g_f}\left(\frac{-c}{a^2}\right) + g_e\left(\frac{1}{b}\right) + g_d(e^{\boxed{a}})$
- $g_x = \frac{\partial y}{\partial x} = \frac{\partial y}{\partial b}\frac{\partial b}{\partial x} + \frac{\partial y}{\partial a}\frac{\partial a}{\partial x} = g_b\left(\frac{1}{x}\right) + g_a(z)$
- $g_z = \frac{\partial y}{\partial z} = \frac{\partial y}{\partial a}\frac{\partial a}{\partial z} = g_a(x)$

Algorithm

BACKPROPAGATION FOR BINARY LOGISTIC REGRESSION

Backpropagation



Case 1:
Logistic
Regression

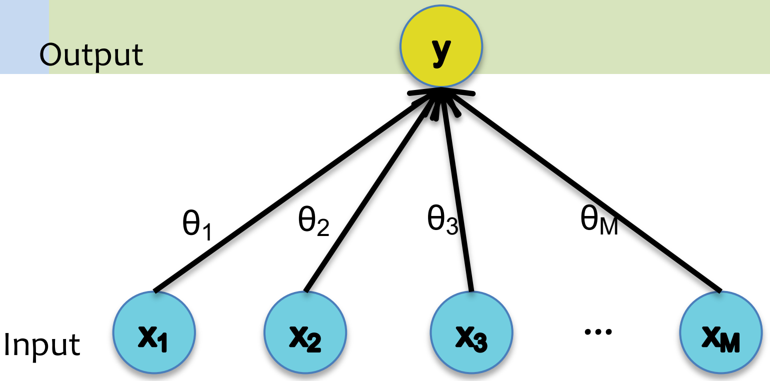
Forward

$$J = y^* \log y + (1 - y^*) \log(1 - y)$$

$$y = \frac{1}{1 + \exp(-a)} = \sigma(a)$$

$$a = \sum_{j=0}^{D} \theta_j x_j = \vec{\theta}^T \vec{x}$$

Backpropagation



Case 1:
Logistic
Regression

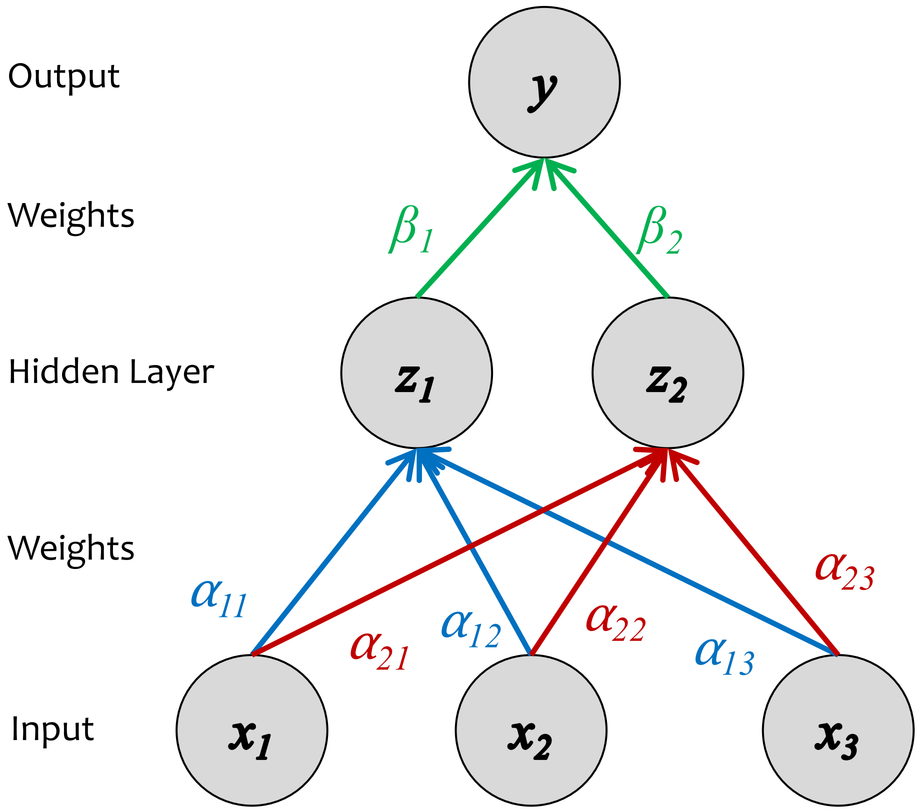
$g_J = \frac{\partial J}{\partial J} = 1$

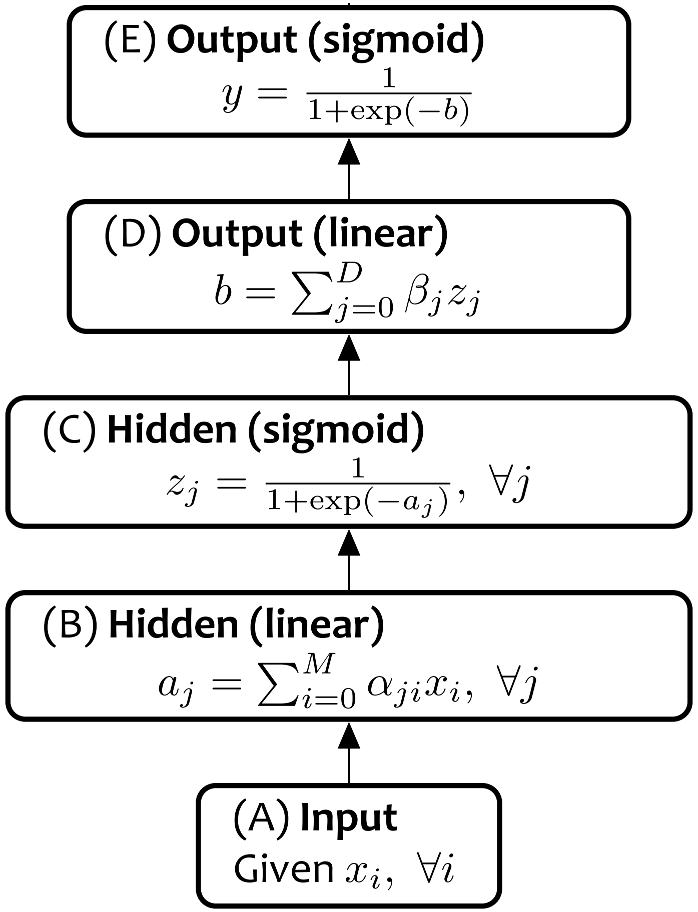
Forward	Backward
$J = y^* \log y + (1 - y^*) \log(1 - y)$	$g_y = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1} = \partial J / \partial y$
$y = \frac{1}{1 + \exp(-a)}$ $\frac{\partial J}{\partial a}$	$g_a = g_y \frac{\partial y}{\partial a}, \frac{\partial y}{\partial a} = \frac{\exp(-a)}{(\exp(-a) + 1)^2}$
$a = \sum_{j=0}^{D} \theta_j x_j$	$g_{\theta_j} = g_a \frac{\partial a}{\partial \theta_j}, \frac{\partial a}{\partial \theta_j} = x_j$ | $g_{\theta_j} = g_a x_j$
	$g_{x_j} = g_a \frac{\partial a}{\partial x_j}, \frac{\partial a}{\partial x_j} = \theta_j$

A 1-Hidden Layer Neural Network

TRAINING / FORWARD COMPUTATION / BACKWARD COMPUTATION

Training Forward-Computation





(E) **Output (sigmoid)**
$y = \frac{1}{1+\exp(-b)}$

(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

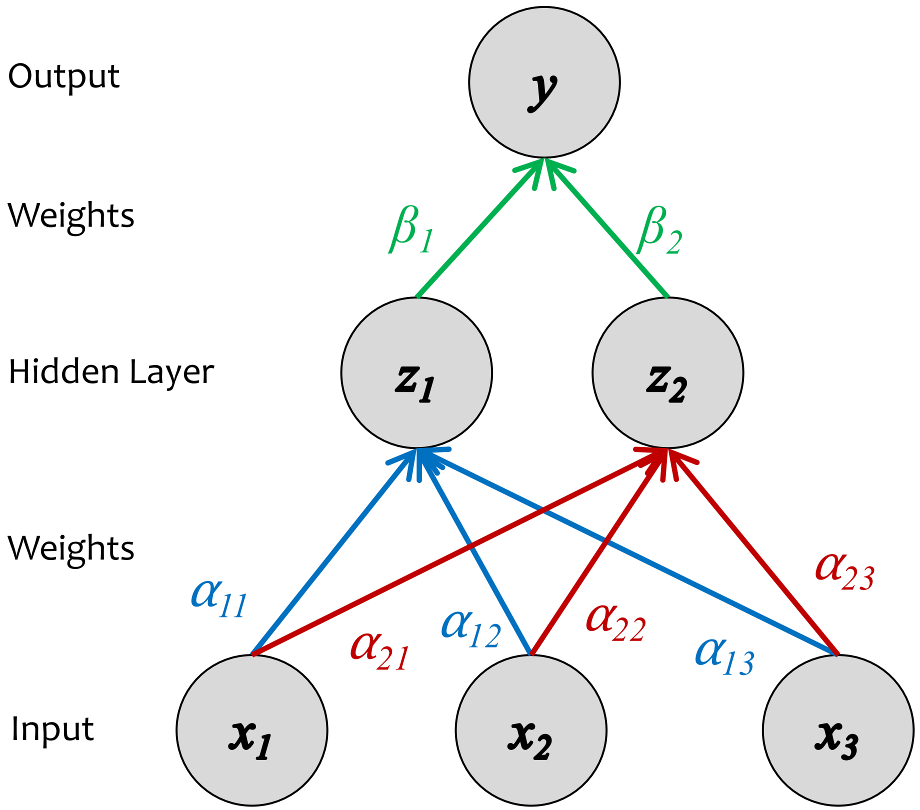
(C) **Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) **Input**
Given $x_i, \ \forall i$

Training

Forward-Computation



cross ent.

(F) **Loss**
$J = \frac{1}{2}(y - y^*)^2$

(E) **Output (sigmoid)**
$y = \frac{1}{1+\exp(-b)}$

(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

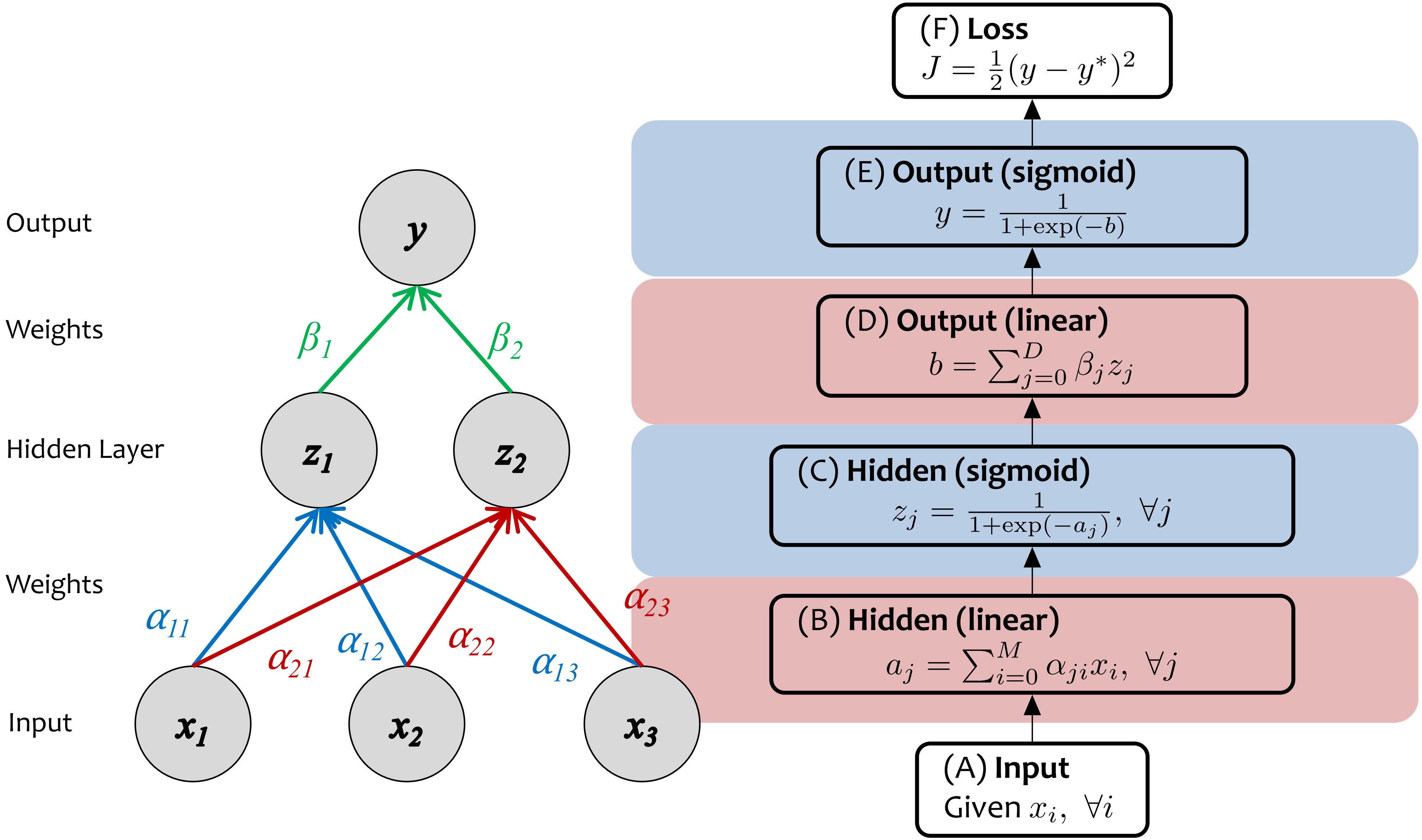
(C) **Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) **Input**
Given $x_i, \ \forall i$

Training

Forward-Computation



(F) **Loss**
$J = \frac{1}{2}(y - y^*)^2$

(E) **Output (sigmoid)**
$y = \frac{1}{1+\exp(-b)}$

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$b = \sum_{j=0}^{D} \beta_j z_j$

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$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) **Input**
Given $x_i, \ \forall i$

Training

SGD with Backprop

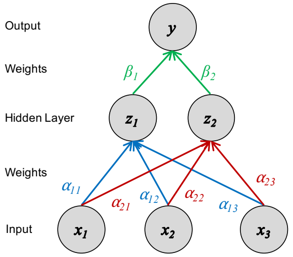
Example: 1-Hidden Layer Neural Network

Algorithm 1 Stochastic Gradient Descent (SGD)

```
procedure SGD(Training data $\mathcal{D}$, ~~test~~ val data $\mathcal{D}_t$)
    Initialize parameters $[\boldsymbol{\alpha}, \boldsymbol{\beta}] = \theta$
    for $e \in \{1, 2, \ldots, E\}$ do
        for $(\mathbf{x}, \mathbf{y}) \in \mathcal{D}$ do
            Compute neural network layers:
            $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{b}, \mathbf{z}, \hat{\mathbf{y}}, J) = \text{NNFORWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta})$
            Compute gradients via backprop:
  $g_\theta$  $\left.\begin{array}{l}\mathbf{g}_{\boldsymbol{\alpha}} = \nabla_{\boldsymbol{\alpha}} J \\ \mathbf{g}_{\boldsymbol{\beta}} = \nabla_{\boldsymbol{\beta}} J\end{array}\right\} = \text{NNBACKWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{o})$
            Update parameters:
            $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha} - \gamma \mathbf{g}_{\boldsymbol{\alpha}}$    $\theta \leftarrow \theta - \gamma g_\theta$
            $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \gamma \mathbf{g}_{\boldsymbol{\beta}}$
        Evaluate training mean cross-entropy $J_{\mathcal{D}}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
        Evaluate ~~test~~ val mean cross-entropy $J_{\mathcal{D}_t}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
    return parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$
```

Backpropagation

Case 2: Neural Network



Forward

$$J = y^* \log y + (1 - y^*) \log(1 - y)$$

$$y = \frac{1}{1 + \exp(-b)}$$

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

Backward

$$g_y = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

$$g_b = g_y \frac{\partial y}{\partial b}, \; \frac{\partial y}{\partial b} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$$

$$g_{\beta_j} = g_b \frac{\partial b}{\partial \beta_j}, \; \frac{\partial b}{\partial \beta_j} = z_j$$

$$g_{z_j} = g_b \frac{\partial b}{\partial z_j}, \; \frac{\partial b}{\partial z_j} = \beta_j$$

$$g_{a_j} = g_{z_j} \frac{\partial z_j}{\partial a_j}, \; \frac{\partial z_j}{\partial a_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$$

$$g_{\alpha_{ji}} = g_{a_j} \frac{\partial a_j}{\partial \alpha_{ji}}, \; \frac{\partial a_j}{\partial \alpha_{ji}} = x_i$$

$$g_{x_i} = \sum_{j=0}^{D} g_{a_j} \frac{\partial a_j}{\partial x_i}, \; \frac{\partial a_j}{\partial x_i} = \alpha_{ji}$$

Training

Backpropagation

Case 2:

	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$g_y = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$g_b = g_y \frac{\partial y}{\partial b}, \; \frac{\partial y}{\partial b} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$g_{\beta_j} = g_b \frac{\partial b}{\partial \beta_j}, \; \frac{\partial b}{\partial \beta_j} = z_j$ $g_{z_j} = g_b \frac{\partial b}{\partial z_j}, \; \frac{\partial b}{\partial z_j} = \beta_j$
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$g_{a_j} = g_{z_j} \frac{\partial z_j}{\partial a_j}, \; \frac{\partial z_j}{\partial a_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$
Linear	$\boxed{a_j} = \sum_{i=0}^{M} \alpha_{ji} x_i$	$g_{\alpha_{ji}} = g_{a_j} \frac{\partial a_j}{\partial \alpha_{ji}}, \; \frac{\partial a_j}{\partial \alpha_{ji}} = x_i$ $g_{x_i} = \sum_{j=0}^{D} g_{a_j} \frac{\partial a_j}{\partial x_i}, \; \frac{\partial a_j}{\partial x_i} = \alpha_{ji}$

Training

Backpropagation

Case 2:	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$\boxed{\frac{dJ}{dy}} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$\boxed{\frac{dJ}{db}} = \boxed{\frac{dJ}{dy}} \frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$\frac{dJ}{d\beta_j} = \boxed{\frac{dJ}{db}} \frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$ $\frac{dJ}{dz_j} = \boxed{\frac{dJ}{db}} \frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$\frac{dJ}{da_j} = \frac{dJ}{dz_j} \frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$
Linear	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j} \frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$ $\frac{dJ}{dx_i} = \sum_{j=0}^{D} \frac{dJ}{da_j} \frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \alpha_{ji}$

Derivative of a Sigmoid

First suppose that

$$s = \frac{1}{1 + \exp(-b)} \tag{1}$$

To obtain the simplified form of the derivative of a sigmoid.

$$\frac{ds}{db} = \boxed{\frac{\exp(-b)}{(\exp(-b) + 1)^2}} \tag{2}$$

$$= \frac{\exp(-b) + 1 - 1}{(\exp(-b) + 1 + 1 - 1)^2} \tag{3}$$

$$= \frac{\exp(-b) + 1 - 1}{(\exp(-b) + 1)^2} \tag{4}$$

$$= \frac{\exp(-b) + 1}{(\exp(-b) + 1)^2} - \frac{1}{(\exp(-b) + 1)^2} \tag{5}$$

$$= \frac{1}{(\exp(-b) + 1)} - \frac{1}{(\exp(-b) + 1)^2} \tag{6}$$

$$= \frac{1}{(\exp(-b) + 1)} - \left(\frac{1}{(\exp(-b) + 1)} \frac{1}{(\exp(-b) + 1)} \right) \tag{7}$$

$$= \frac{1}{(\exp(-b) + 1)} \left(1 - \frac{1}{(\exp(-b) + 1)} \right) \tag{8}$$

$$\boxed{= s(1 - s)} \tag{9}$$

Backpropagation

Case 2:	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$g_y = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$g_b = g_y \frac{\partial y}{\partial b}, \boxed{\frac{\partial y}{\partial b} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}}$
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$g_{\beta_j} = g_b \frac{\partial b}{\partial \beta_j}, \frac{\partial b}{\partial \beta_j} = z_j$ $g_{z_j} = g_b \frac{\partial b}{\partial z_j}, \frac{\partial b}{\partial z_j} = \beta_j$
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$g_{a_j} = g_{z_j} \frac{\partial z_j}{\partial a_j}, \boxed{\frac{\partial z_j}{\partial a_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}}$
Linear	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$g_{\alpha_{ji}} = g_{a_j} \frac{\partial a_j}{\partial \alpha_{ji}}, \frac{\partial a_j}{\partial \alpha_{ji}} = x_i$ $g_{x_i} = \sum_{j=0}^{D} g_{a_j} \frac{\partial a_j}{\partial x_i}, \frac{\partial a_j}{\partial x_i} = \alpha_{ji}$

Training

Backpropagation

vanishing gradient problem

Case 2:	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$g_y = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$g_b = g_y \frac{\partial y}{\partial b}, \frac{\partial y}{\partial b} = y(1 - y)$ ∈(0,1)
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$g_{\beta_j} = g_b \frac{\partial b}{\partial \beta_j}, \frac{\partial b}{\partial \beta_j} = z_j$ $g_{z_j} = g_b \frac{\partial b}{\partial z_j}, \frac{\partial b}{\partial z_j} = \beta_j$ ∈(0,1)
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$g_{a_j} = \underline{g_{z_j}} \frac{\partial z_j}{\partial a_j}, \frac{\partial z_j}{\partial a_j} = \underline{z_j}\underline{(1 - z_j)}$
Linear	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$g_{\alpha_{ji}} = g_{a_j} \frac{\partial a_j}{\partial \alpha_{ji}}, \frac{\partial a_j}{\partial \alpha_{ji}} = x_i$ $g_{x_i} = \sum_{j=0}^{D} g_{a_j} \frac{\partial a_j}{\partial x_i}, \frac{\partial a_j}{\partial x_i} = \alpha_{ji}$

Training

SGD with Backprop

Example: 1-Hidden Layer Neural Network

Algorithm 1 Stochastic Gradient Descent (SGD)

```
procedure SGD(Training data $\mathcal{D}$, test data $\mathcal{D}_t$)
    Initialize parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$
    for $e \in \{1, 2, \ldots, E\}$ do
        for $(\mathbf{x}, \mathbf{y}) \in \mathcal{D}$ do
            Compute neural network layers:
            $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{b}, \mathbf{z}, \hat{\mathbf{y}}, J) = \text{NNFORWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta})$
            Compute gradients via backprop:
            $\left.\begin{aligned} \mathbf{g}_{\boldsymbol{\alpha}} &= \nabla_{\boldsymbol{\alpha}} J \\ \mathbf{g}_{\boldsymbol{\beta}} &= \nabla_{\boldsymbol{\beta}} J \end{aligned}\right\} = \text{NNBACKWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{o})$
            Update parameters:
            $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha} - \gamma \mathbf{g}_{\boldsymbol{\alpha}}$
            $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \gamma \mathbf{g}_{\boldsymbol{\beta}}$
        Evaluate training mean cross-entropy $J_{\mathcal{D}}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
        Evaluate test mean cross-entropy $J_{\mathcal{D}_t}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
    return parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$
```

In-Class Poll

Question: Q1

What questions do *you* have?

A 2-Hidden Layer Neural Network

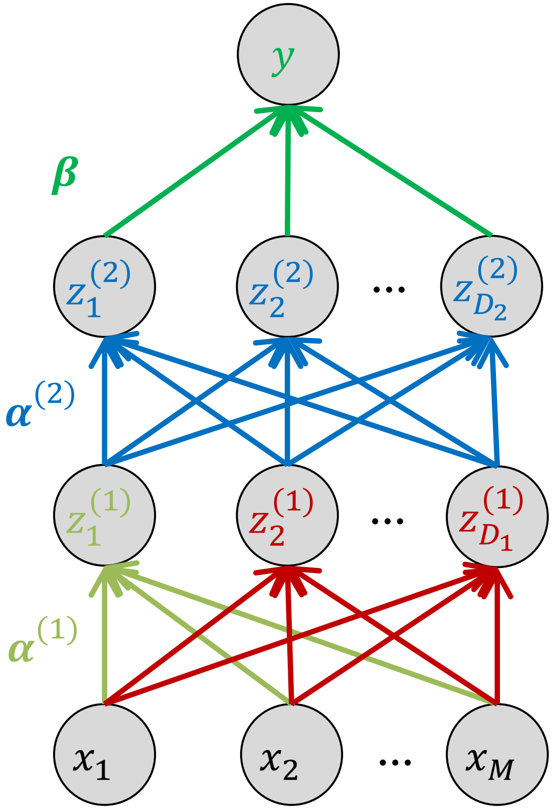
TRAINING / FORWARD COMPUTATION / BACKWARD COMPUTATION

Training

Backpropagation

Recall: Our 2-Hidden Layer Neural Network

Question: How do we train this model?



$\boldsymbol{\beta} \in \mathbb{R}^{D_2}$

$\beta_0 \in \mathbb{R}$

$\boldsymbol{\alpha}^{(2)} \in \mathbb{R}^{M \times D_2}$

$\boldsymbol{b}^{(2)} \in \mathbb{R}^{D_2}$

$\boldsymbol{\alpha}^{(1)} \in \mathbb{R}^{M \times D_1}$

$\boldsymbol{b}^{(1)} \in \mathbb{R}^{D_1}$

$$y = \sigma((\boldsymbol{\beta})^T \boldsymbol{z}^{(2)} + \beta_0)$$

$$\boldsymbol{z}^{(2)} = \sigma((\boldsymbol{\alpha}^{(2)})^T \boldsymbol{z}^{(1)} + \boldsymbol{b}^{(2)})$$

$$\boldsymbol{z}^{(1)} = \sigma((\boldsymbol{\alpha}^{(1)})^T \boldsymbol{x} + \boldsymbol{b}^{(1)})$$

Example: Neural Net Training (2-Hidden Layers)

- Consider a 2-hidden layer NN
- params. are $\Theta = [\alpha^{(1)}, \alpha^{(2)}, \beta]$
- SGD Training

Iterate until convergence:

① Sample $i \sim \text{Unif}(1, \dots, N)$

② Compute gradient by backprop:

$$g_{\alpha^{(1)}} = \nabla_{\alpha^{(1)}} J^{(i)}(\Theta) = \partial J^{(i)}(\Theta) / \partial \alpha^{(1)}$$

$$g_{\alpha^{(2)}} = \nabla_{\alpha^{(2)}} J^{(i)}(\Theta) = \partial J \cdots / \partial \alpha^{(2)}$$

$$g_{\beta} = \nabla_{\beta} J^{(i)}(\Theta) = \partial J \cdots / \partial \beta$$

$$J^{(i)}(\Theta) = \text{loss}(h_\Theta(\vec{x}^{(i)}), y^{(i)})$$

③ Update parameters

$$\alpha^{(1)} \leftarrow \alpha^{(1)} - \gamma g_{\alpha^{(1)}}$$

$$\alpha^{(2)} \leftarrow \alpha^{(2)} - \gamma g_{\alpha^{(2)}}$$

$$\beta \leftarrow \beta - \gamma g_{\beta}$$

Background

$$\nabla J(\vec{a}, \vec{b}) = \nabla_{\vec{a}, \vec{b}} J(\vec{a}, \vec{b})$$

$$\nabla_{\vec{a}} J(\vec{a}, \vec{b}) = \begin{bmatrix} \partial J / \partial a_1 \\ \partial J / \partial a_2 \\ \vdots \\ \partial J / \partial a_K \end{bmatrix} = \frac{\partial J}{\partial \vec{a}}$$

$$|\vec{a}| = K$$

Example: Backpropagation (2-Hidden Layers)

Given:

① Dec. fn. $$\hat{y} = h_\theta(\vec{x}) = \sigma\Big(\underbrace{(\alpha^{(3)})^T}_{\beta} \underbrace{\sigma\big((\alpha^{(2)})^T \underbrace{\sigma((\alpha^{(1)})^T\vec{x})}_{\vec{z}^{(1)}}\big)}_{\vec{z}^{(2)}}\Big)$$

left out the intercept terms

② Loss fn. $J = \ell(\hat{y}, y^*) = -(y^*\log(\hat{y}) + (1-y^*)\log(1-\hat{y}))$

③ Training ex. $(\vec{x}, y^*)$

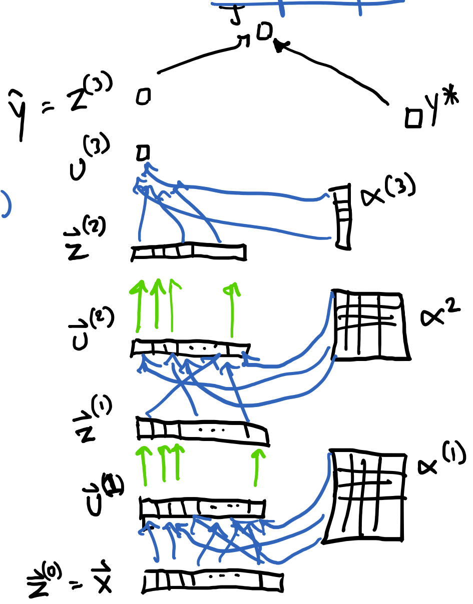
Forward Comp.

Given $\vec{x}, y^*, \alpha^{(1)}, \alpha^{(2)}, \alpha^{(3)}$

$\vec{z}^{(0)} = \vec{x}$

```
for i = 1,2,3:
    $\vec{u}^{(i)} = (\alpha^{(i)})^T \vec{z}^{(i-1)}$
    $\vec{z}^{(i)} = \sigma(\vec{u}^{(i)})$
$\hat{y} = \vec{z}^{(3)}$
$J = \ell(\hat{y}, y^*)$
```

Comp Graph



Backward Comp.

$g_J = [1]$

$g_{\hat{y}} = -\left(\frac{y^*}{\hat{y}} - \frac{(1-y^*)}{1-\hat{y}}\right)$

$g_{z^{(3)}} = g_{\hat{y}}$

```
for i = 3,2,1:
    $g_{u^{(i)}} = \ldots$
    $g_{\alpha^{(i)}} = \ldots$
    $g_{z^{(i-1)}} = \ldots$
$g_{\vec{x}} = g_{\vec{z}^{(0)}}$
```

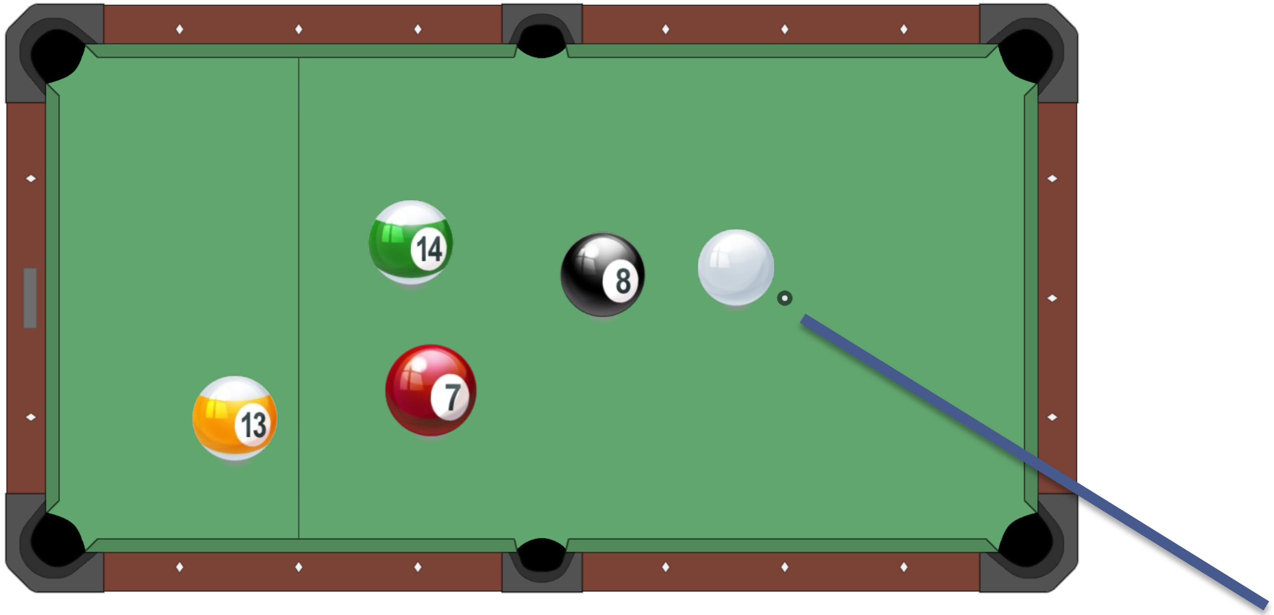
HWS

Example: Backpropagation (2-Hidden Layers)

Intuitions

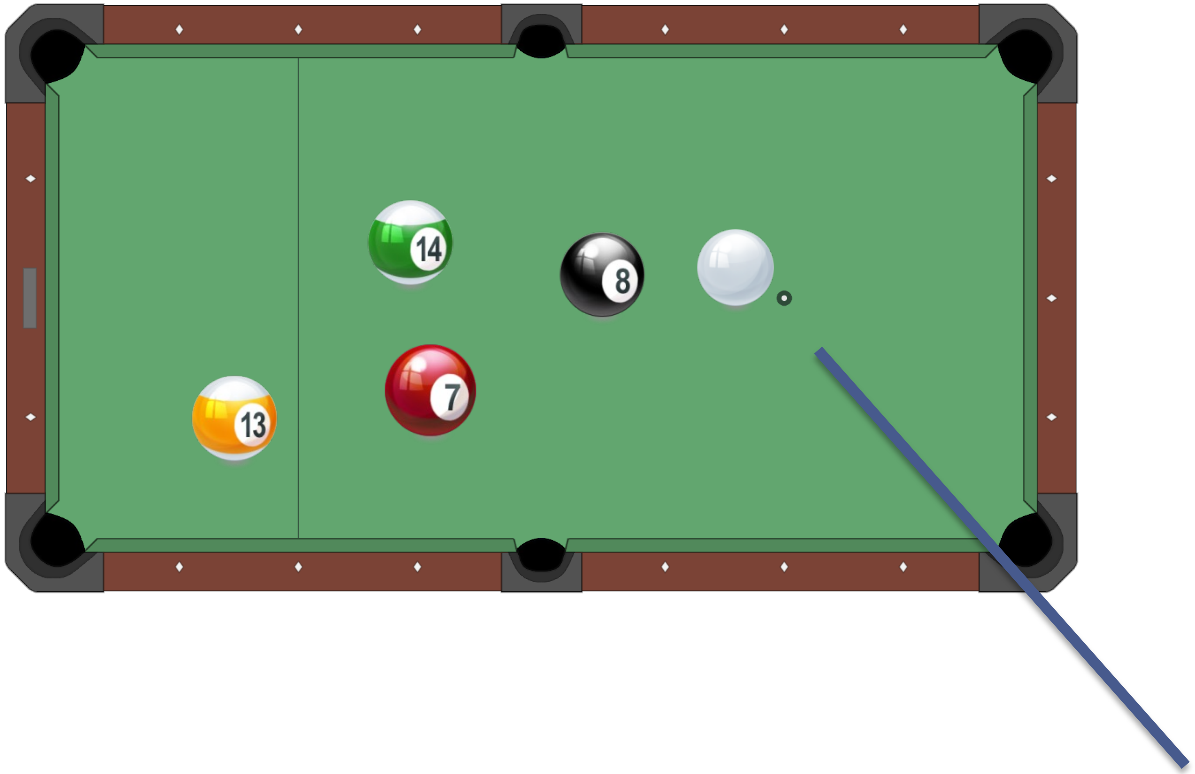
BACKPROPAGATION OF ERRORS

Error Back-Propagation



Slide from (Stoyanov & Eisner, 2012)

Error Back-Propagation



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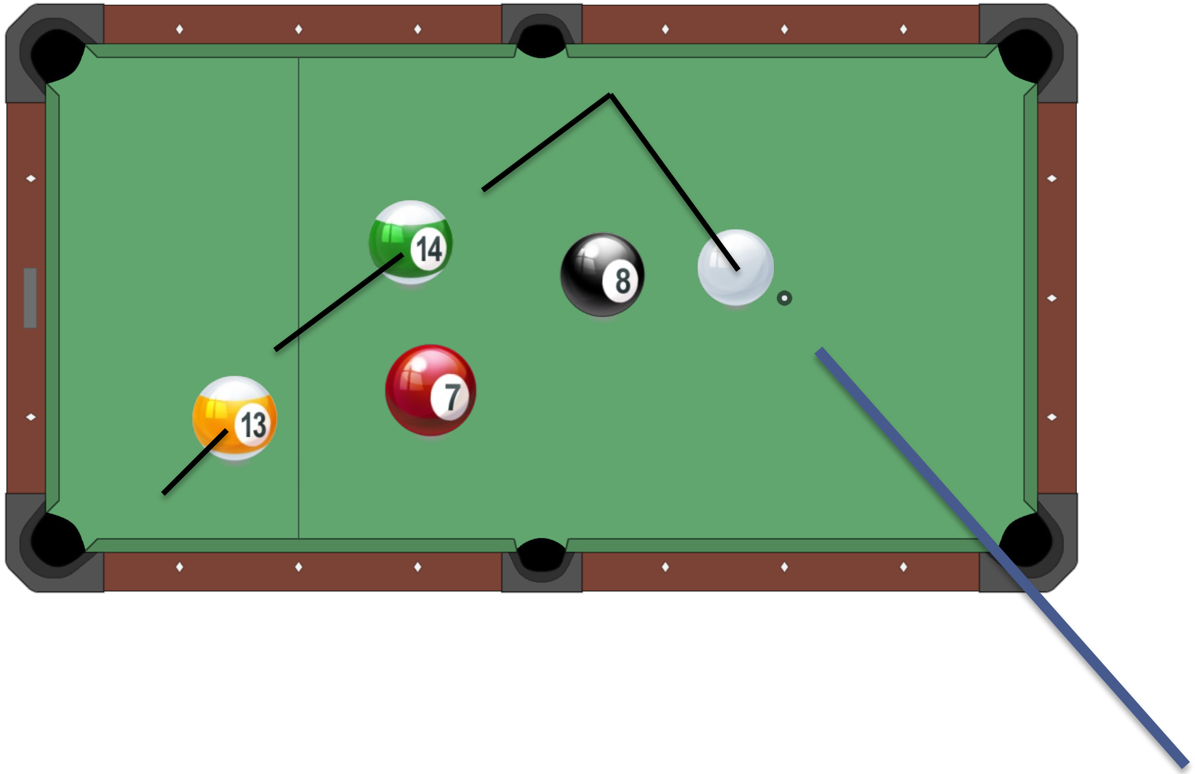

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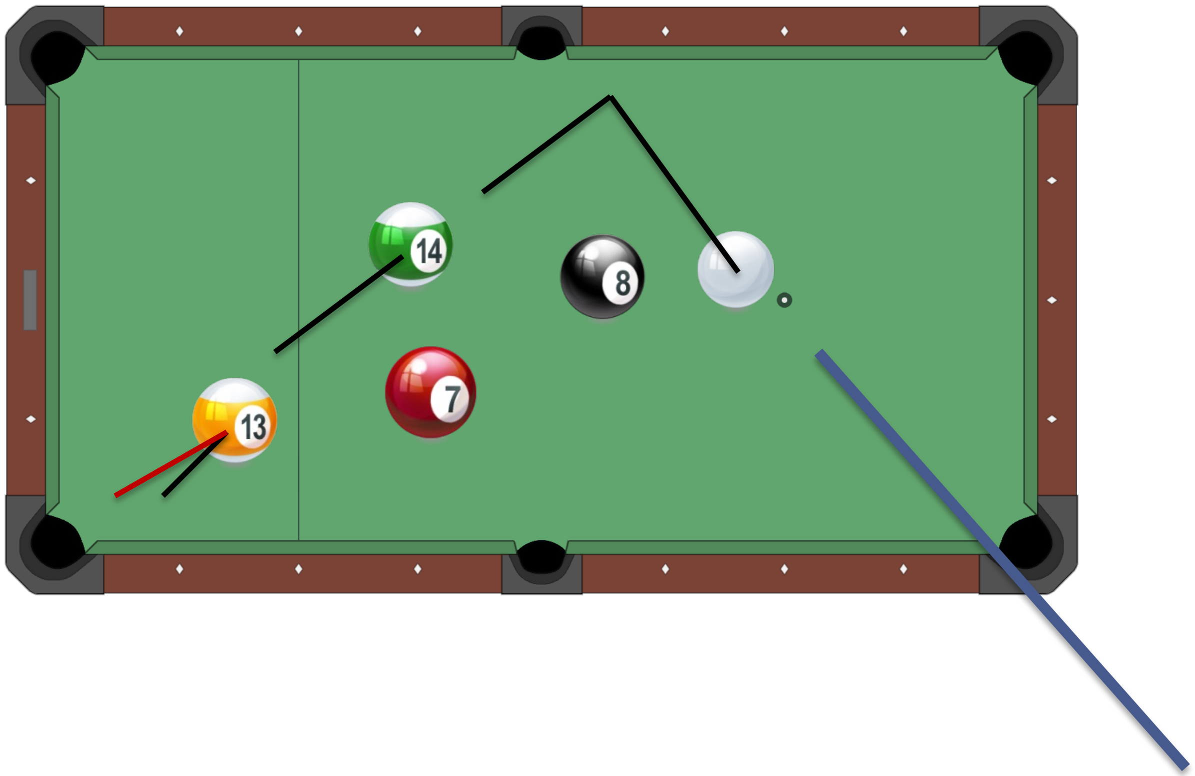

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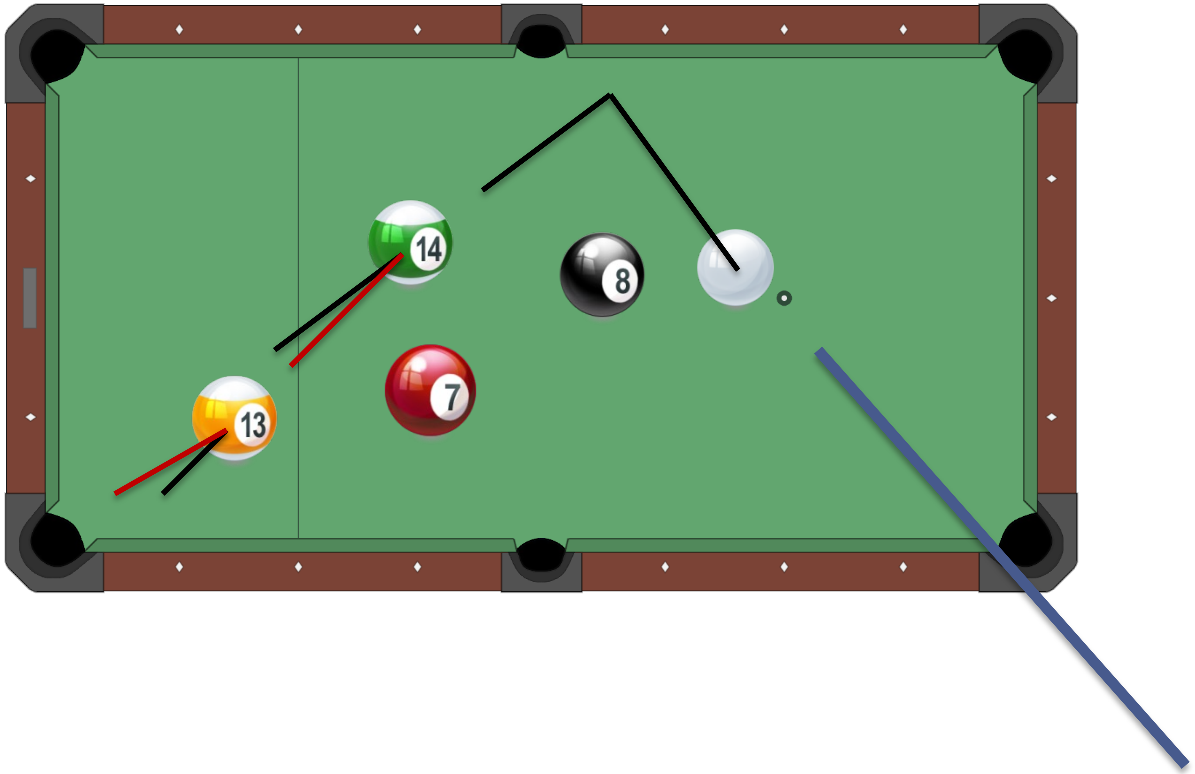

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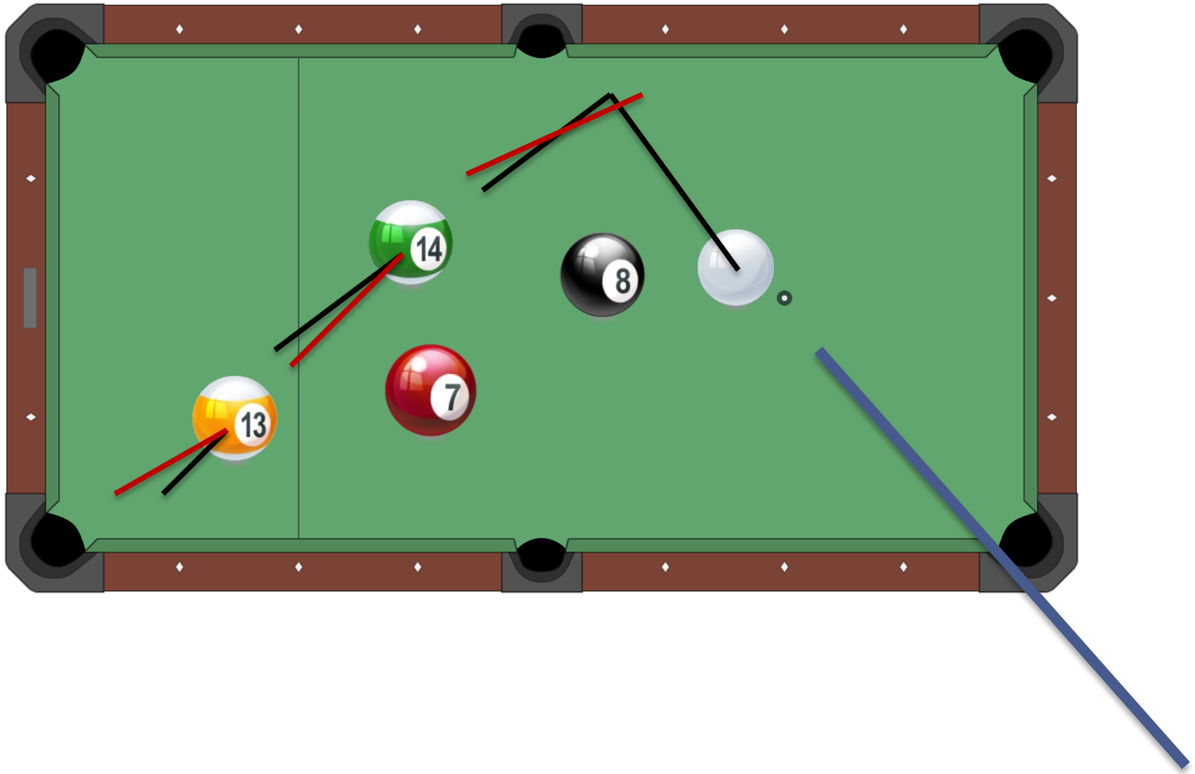

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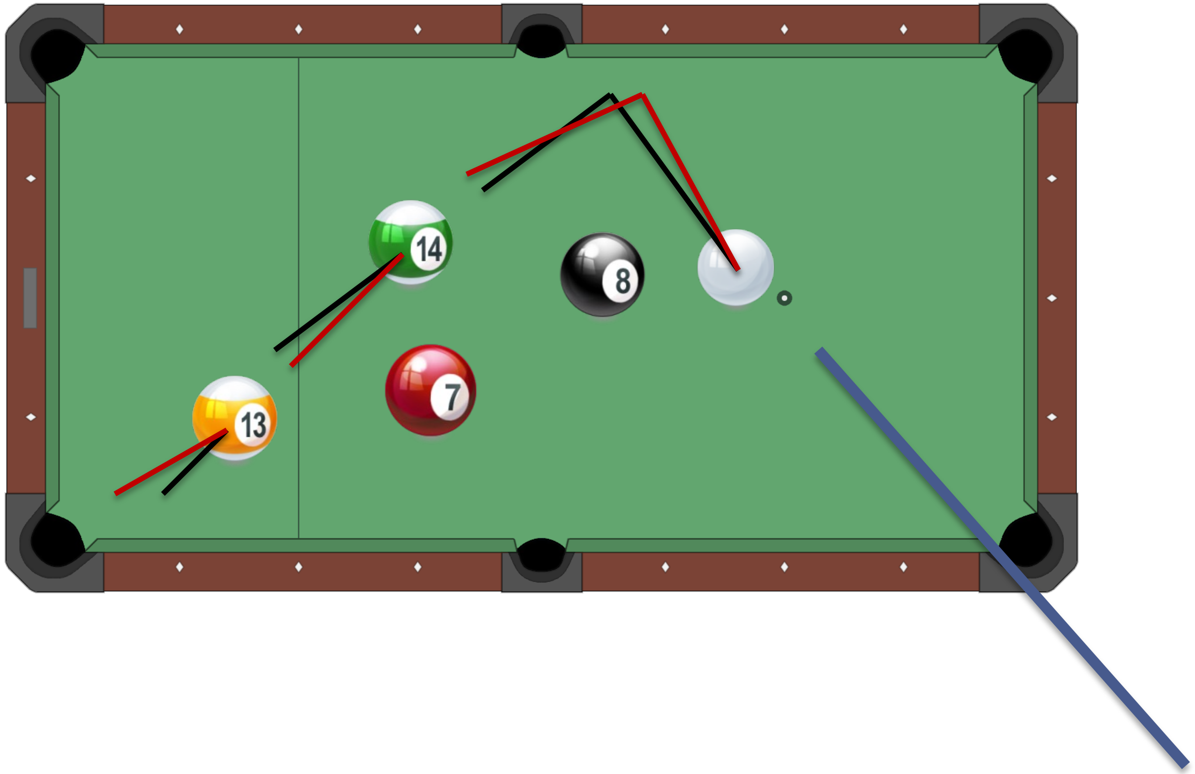

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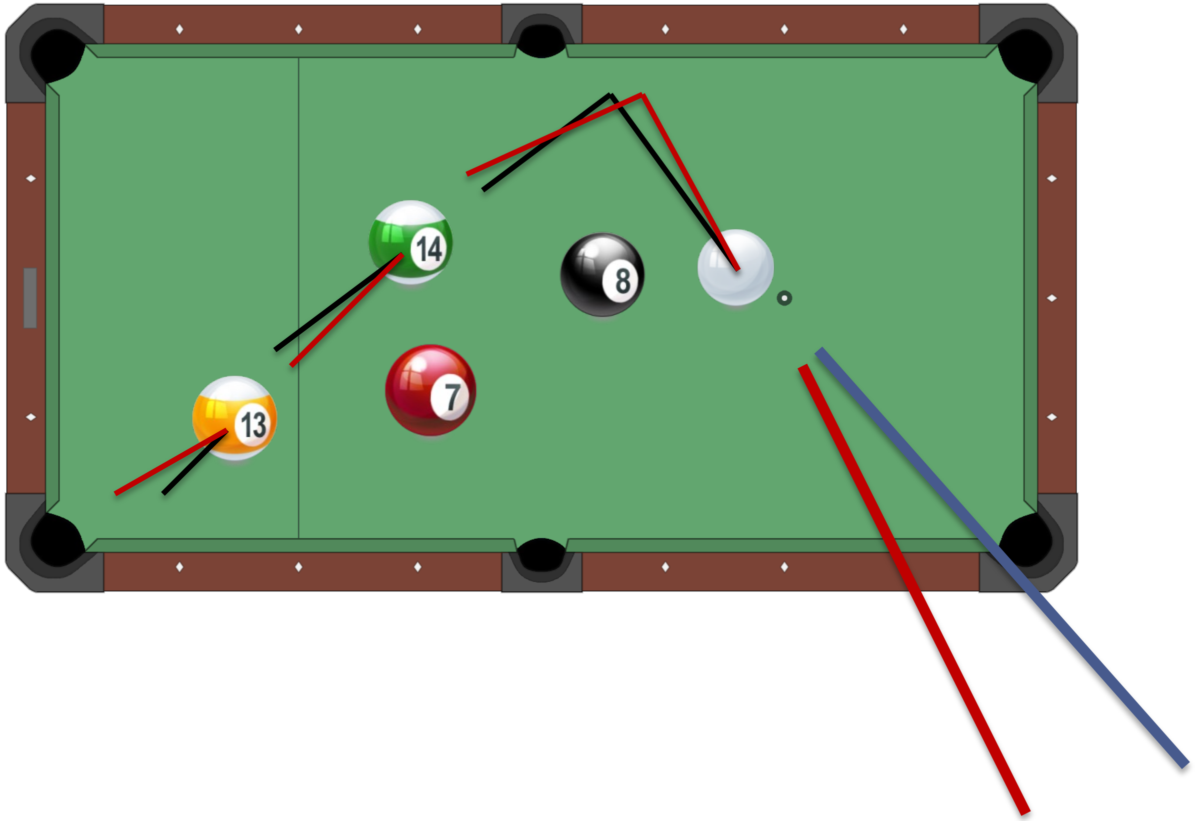

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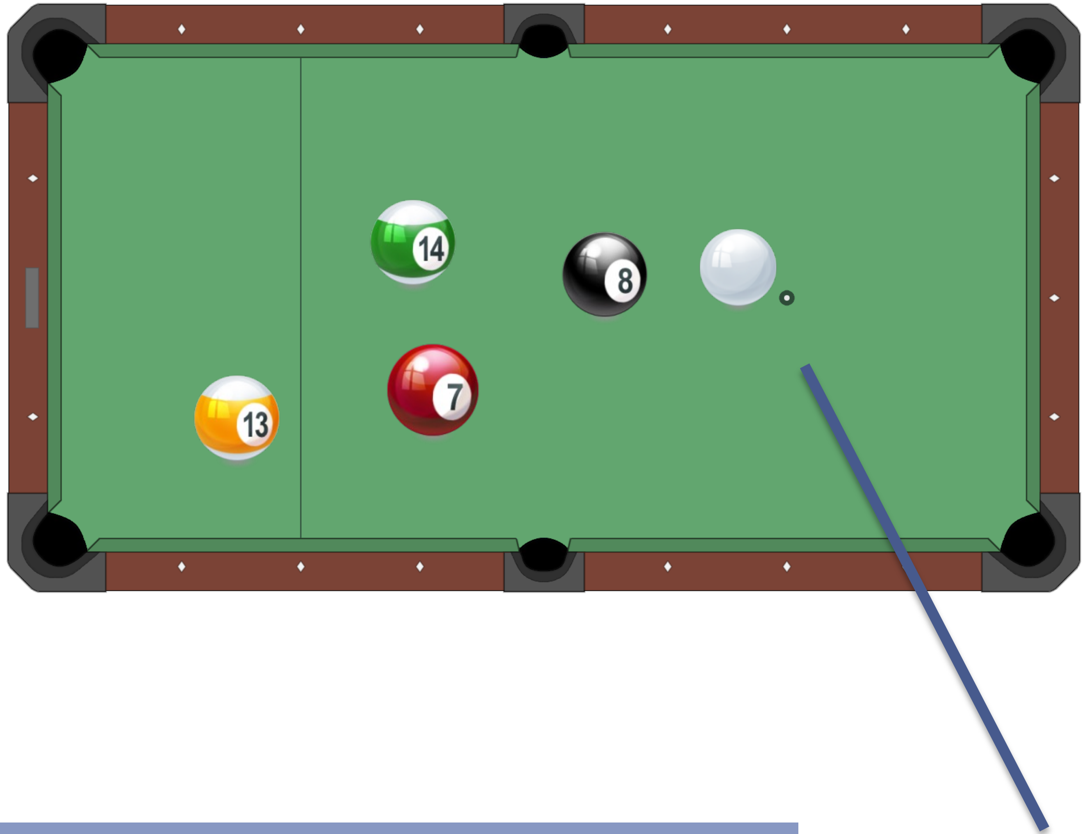

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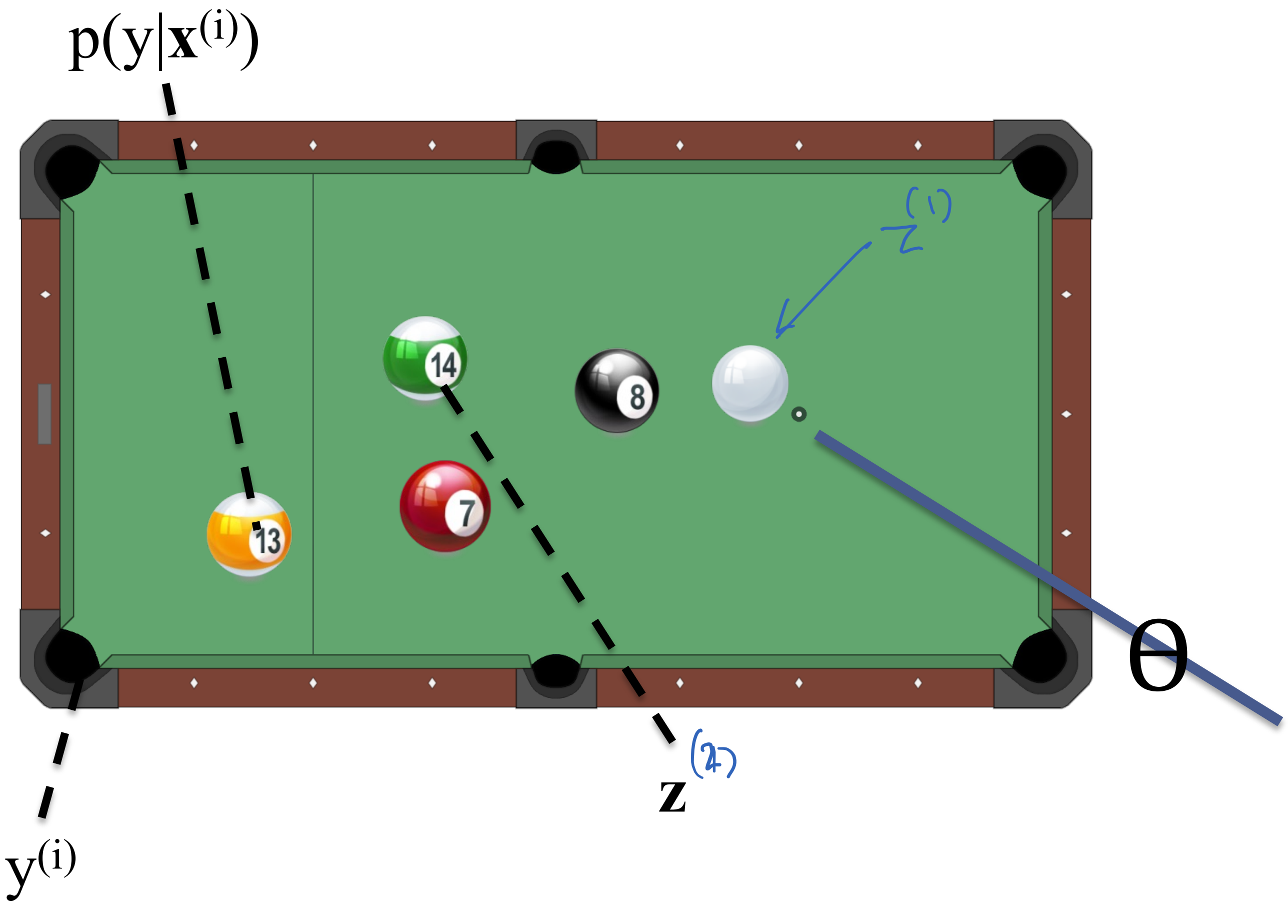

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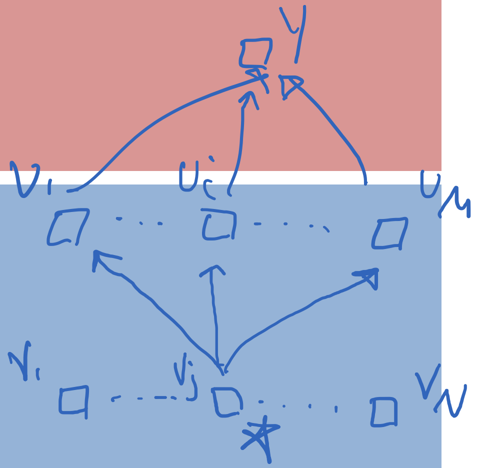
THE BACKPROPAGATION ALGORITHM

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

<u>Forward Computation</u>

1. Write an **algorithm** for evaluating the function y = f(**x**). The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph**")
2. Visit each node in **topological order**.
   For variable u_i with inputs $v_1, \dots, v_N$
   a. Compute $u_i = g_i(v_1, \dots, v_N)$
   b. Store the result at the node



<u>Backward Computation (Version A)</u>

1. **Initialize** dy/dy = 1.
2. Visit each node v_j in **reverse topological order**.
   Let $u_1, \dots, u_M$ denote all the nodes with v_j as an input
   Assuming that y = h(**u**) = h($u_1, \dots, u_M$)
   and **u** = g(**v**) or equivalently $u_i = g_i(v_1, \dots, v_j, \dots, v_N)$ for all i
   a. We already know dy/du_i for all i
   b. Compute dy/dv_j as below (Choice of algorithm ensures computing (du_i/dv_j) is easy)

$$\frac{dy}{dv_j} = \sum_{i=1}^{M} \frac{dy}{du_i}\frac{du_i}{dv_j}$$

Return partial derivatives dy/du_i for all variables

Training

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

<u>Forward Computation</u>

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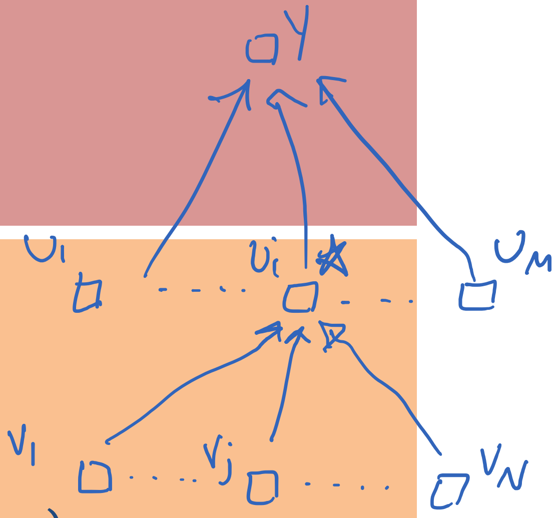
   a. Compute $u_i = g_i(v_1,\dots, v_N)$
   b. Store the result at the node

<u>Backward Computation (Version B)</u> g_{u_j} g_y

1. **Initialize** all partial derivatives dy/du_j to 0 and $dy/dy = 1$.
2. Visit each node in **reverse topological order**.
   For variable $u_i = g_i(v_1,\dots, v_N)$
   a. We already know dy/du_i
   b. Increment $\boxed{dy/dv_j}$ by $\boxed{(dy/du_i)(du_i/dv_j)}$
   (Choice of algorithm ensures computing (du_i/dv_j) is easy)



Return partial derivatives dy/du_i for all variables

Training

Backpropagation (Version B)

Simple Example: The goal is to compute $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative $\frac{dJ}{dx}$ on the backward pass.

Forward

$J = \cos(u)$

$u = u_1 + u_2$

$u_1 = \sin(t)$

$u_2 = 3t$

$t = x^2$

Backpropagation (Version B)

Simple Example: The goal is to compute $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative $\frac{dJ}{dx}$ on the backward pass.

$g_u = 0, g_{u_1} = 0, g_{u_2} = 0, g_t = 0, g_x = 0$, $g_J = 1$

Initialize all the adjoints to zero

Forward	Backward
$J = \cos(u)$	$g_u \mathrel{+}= -\sin(u)$
$u = u_1 + u_2$	$g_{u_1} \mathrel{+}= g_u \frac{du}{du_1}, \quad \frac{du}{du_1} = 1 \qquad g_{u_2} \mathrel{+}= g_u \frac{du}{du_2}, \quad \frac{du}{du_2} = 1$
$u_1 = \sin(t)$	$g_t \mathrel{+}= g_{u_1} \frac{du_1}{dt}, \quad \frac{du_1}{dt} = \cos(t)$
$u_2 = 3t$	$g_t \mathrel{+}= g_{u_2} \frac{du_2}{dt}, \quad \frac{du_2}{dt} = 3$
$t = x^2$	$g_x \mathrel{+}= g_t \frac{dt}{dx}, \quad \frac{dt}{dx} = 2x$

$g_t = g_{u_1} \frac{du_1}{dt} + g_{u_2} \frac{du_2}{dt}$

Notice that we increment the partial derivative for $\frac{dJ}{dt}$ in two places!

Backpropagation

Why is the backpropagation algorithm efficient?

1. Reuses **computation from the forward pass** in the backward pass
2. Reuses **partial derivatives** throughout the backward pass (*but only if the algorithm reuses shared computation in the forward pass*)

   (Key idea: partial derivatives in the backward pass should be thought of as variables stored for reuse)

Background

A Recipe for

Gradients

Backpropagation can compute this gradient!

And it's a **special case of a more general algorithm** called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

1. Given training dat

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of t

– Decision functio

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

$\boldsymbol{y}_i)$

opposite the gradient)

$$\boldsymbol{\theta}^{(t} \quad {}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

MATRIX CALCULUS

Q&A

Q: Do I need to know **matrix calculus** to derive the backprop algorithms used in this class?

A: Well, we've carefully constructed our assignments so that you do **not** need to know matrix calculus.

That said, it's pretty handy. So we *added matrix calculus to our learning objectives* for backprop.

Matrix Calculus

Let $y, x \in \mathbb{R}$ be scalars, $\mathbf{y} \in \mathbb{R}^M$ and $\mathbf{x} \in \mathbb{R}^P$ be vectors, and $\mathbf{Y} \in \mathbb{R}^{M \times N}$ and $\mathbf{X} \in \mathbb{R}^{P \times Q}$ be matrices

Numerator

Denominator

Types of Derivatives	**scalar**	**vector**	**matrix**
scalar	$\frac{\partial y}{\partial x}$	$\frac{\partial \mathbf{y}}{\partial x}$	$\frac{\partial \mathbf{Y}}{\partial x}$
vector	$\frac{\partial y}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{Y}}{\partial \mathbf{x}}$
matrix	$\frac{\partial y}{\partial \mathbf{X}}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{X}}$	$\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}$

Matrix Calculus

Types of Derivatives	**scalar**
scalar	$\frac{\partial y}{\partial x} = \left[\frac{\partial y}{\partial x}\right]$
vector	$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix}$
matrix	$\frac{\partial y}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial y}{\partial X_{11}} & \frac{\partial y}{\partial X_{12}} & \cdots & \frac{\partial y}{\partial X_{1Q}} \\ \frac{\partial y}{\partial X_{21}} & \frac{\partial y}{\partial X_{22}} & \cdots & \frac{\partial y}{\partial X_{2Q}} \\ \vdots & & & \vdots \\ \frac{\partial y}{\partial X_{P1}} & \frac{\partial y}{\partial X_{P2}} & \cdots & \frac{\partial y}{\partial X_{PQ}} \end{bmatrix}$

Matrix Calculus

Types of Derivatives	**scalar**	**vector**
scalar	$\frac{\partial y}{\partial x} = \left[\frac{\partial y}{\partial x}\right]$	$\frac{\partial \mathbf{y}}{\partial x} = \left[\frac{\partial y_1}{\partial x} \quad \frac{\partial y_2}{\partial x} \quad \cdots \quad \frac{\partial y_N}{\partial x}\right]$
vector	$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_N}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_N}{\partial x_2} \\ \vdots & & & \\ \frac{\partial y_1}{\partial x_P} & \frac{\partial y_2}{\partial x_P} & \cdots & \frac{\partial y_N}{\partial x_P} \end{bmatrix}$

Matrix Calculus

Whenever you read about matrix calculus, you'll be confronted with two layout conventions:

Let $y, x \in \mathbb{R}$ be scalars, $\mathbf{y} \in \mathbb{R}^M$ and $\mathbf{x} \in \mathbb{R}^P$ be vectors.

1. In numerator layout:

$$\frac{\partial y}{\partial \mathbf{x}} \text{ is a } 1 \times P \text{ matrix, i.e. a row vector}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \text{ is an } M \times P \text{ matrix}$$

2. In denominator layout:

$$\frac{\partial y}{\partial \mathbf{x}} \text{ is a } P \times 1 \text{ matrix, i.e. a column vector}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \text{ is an } P \times M \text{ matrix}$$

In this course, **we use denominator layout**.

Why? This ensures that our gradients of the objective function with respect to some subset of parameters are the same shape as those parameters.

Vector Derivatives

$$\frac{\partial \vec{x}^T\vec{x}}{\partial \vec{x}} = 2x = \begin{bmatrix} \partial f/dx_1 \\ \vdots \\ \partial f/dx_m \end{bmatrix}$$

Scalar Derivatives

Suppose $x \in \mathbb{R}$
and $f : \mathbb{R} \to \mathbb{R}$

$f(x)$	$\frac{\partial f(x)}{\partial x}$
bx	b
xb	b
x^2	$2x$
bx^2	$2bx$

Vector Derivatives

Suppose $\mathbf{x} \in \mathbb{R}^m$, $\mathbf{b} \in \mathbb{R}^m$,
$\mathbf{B} \in \mathbb{R}^{m \times n}$, $\mathbf{Q} \in \mathbb{R}^{m \times m}$
and $\mathbf{Q}$ is symmetric.

$f(\mathbf{x})$	$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$	type of f
→ $\mathbf{b}^T\mathbf{x}$	$\mathbf{b}$	$f : \mathbb{R}^m \to \mathbb{R}$
$\mathbf{x}^T\mathbf{b}$	$\mathbf{b}$	$f : \mathbb{R}^m \to \mathbb{R}$
$\mathbf{x}^T\mathbf{B}$	$\mathbf{B}$	$f : \mathbb{R}^m \to \mathbb{R}^n$
$\mathbf{B}^T\mathbf{x}$	$\mathbf{B}^T$	$f : \mathbb{R}^m \to \mathbb{R}^n$
$\mathbf{x}^T\mathbf{x}$	$2\mathbf{x}$	$f : \mathbb{R}^m \to \mathbb{R}$
$\mathbf{x}^T\mathbf{Q}\mathbf{x}$	$2\mathbf{Q}\mathbf{x}$	$f : \mathbb{R}^m \to \mathbb{R}$

$$\sum_i x_i^2$$

Vector Derivatives

Scalar Derivatives

Suppose $\mathbf{x} \in \mathbb{R}^m$ and we have constants $a \in \mathbb{R}$, $b \in \mathbb{R}$

$f(x)$	$\frac{\partial f(x)}{\partial x}$
$g(x) + h(x)$	$\frac{\partial g(x)}{\partial x} + \frac{\partial h(x)}{\partial x}$
$ag(x)$	$a\frac{\partial g(x)}{\partial x}$
$g(x)b$	$\frac{\partial g(x)}{\partial x}b$

Vector Derivatives

Suppose $\mathbf{x} \in \mathbb{R}^m$ and we have constants $a \in \mathbb{R}$, $\mathbf{b} \in \mathbb{R}^n$

$f(\mathbf{x})$	$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$
$g(\mathbf{x}) + h(\mathbf{x})$	$\frac{\partial g(\mathbf{x})}{\partial \mathbf{x}} + \frac{\partial h(\mathbf{x})}{\partial \mathbf{x}}$
$ag(\mathbf{x})$	$a\frac{\partial g(\mathbf{x})}{\partial \mathbf{x}}$
$g(\mathbf{x})\mathbf{b}$	$\frac{\partial g(\mathbf{x})}{\partial \mathbf{x}}\mathbf{b}^T$

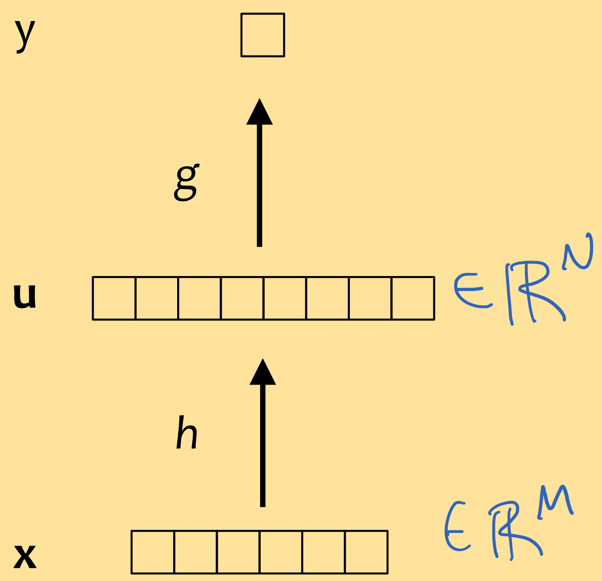
Matrix Calculus

$\underbrace{\frac{\partial y}{\partial u}}_{M \times 1}$

$\frac{\partial u}{\partial x}$ $N \times M$

Question: Q2

Suppose y = g(**u**) and **u** = h(**x**)



Which of the following is the correct definition of the chain rule?

Recall:

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix} \qquad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \dots & \frac{\partial y_N}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_N}{\partial x_2} \\ \vdots & & & \\ \frac{\partial y_1}{\partial x_P} & \frac{\partial y_2}{\partial x_P} & \dots & \frac{\partial y_N}{\partial x_P} \end{bmatrix}$$

Answer:

$$\frac{\partial y}{\partial \mathbf{x}} = \dots$$

A. $\frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

B. $\frac{\partial y}{\partial \mathbf{u}}^T \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

C. $\frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}^T$

D. $\frac{\partial y}{\partial \mathbf{u}}^T \frac{\partial \mathbf{u}}{\partial \mathbf{x}}^T$

E. $(\frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}})^T$

[✓ F. None of the above]

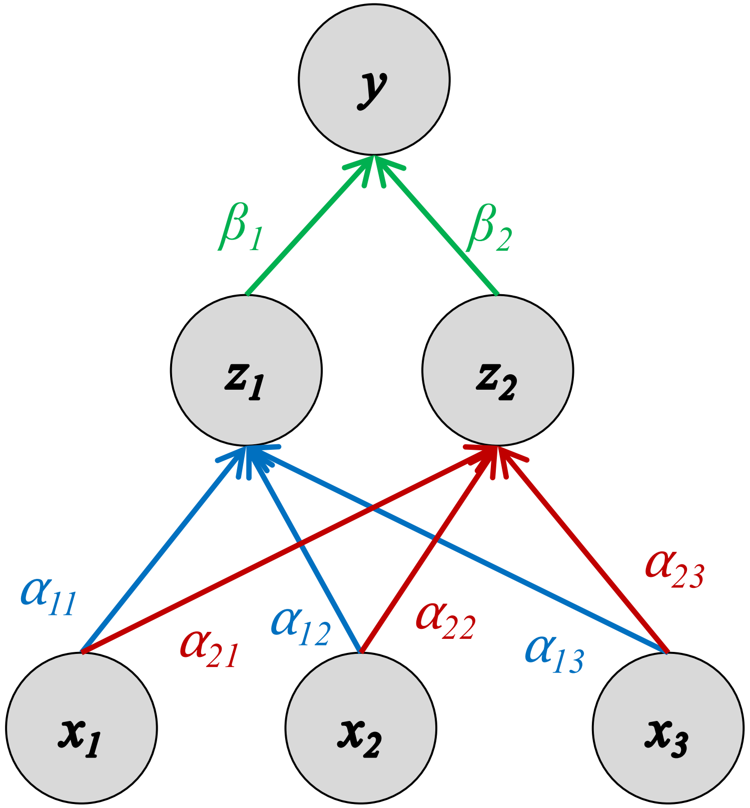
$\frac{\partial u}{\partial x} \frac{\partial y}{\partial u}$

DRAWING A NEURAL NETWORK

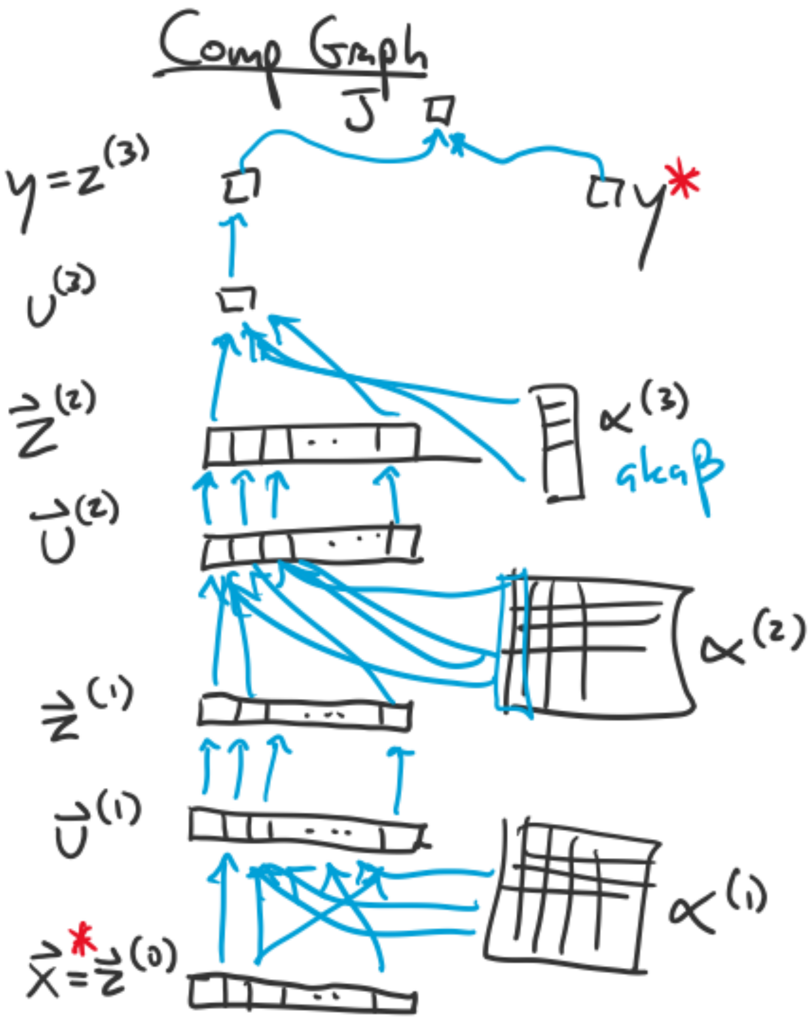
Ways of Drawing Neural Networks

Neural Network Diagram

- The diagram represents a neural network
- Nodes are **circles**
- One node per hidden unit
- Node is labeled with the variable corresponding to the hidden unit
- For a fully connected feed-forward neural network, a hidden unit is a nonlinear function of nodes in the previous layer
- *Edges are directed*
- Each edge is labeled with its weight (side note: we should be careful about ascribing how a matrix can be used to indicate the labels of the edges and pitfalls there)
- Other details:
  - Following standard convention, the intercept term is NOT shown as a node, but rather is assumed to be part of the non-linear function that yields a hidden unit. (i.e. its weight does NOT appear in the picture anywhere)
  - The diagram does NOT include any nodes related to the loss computation



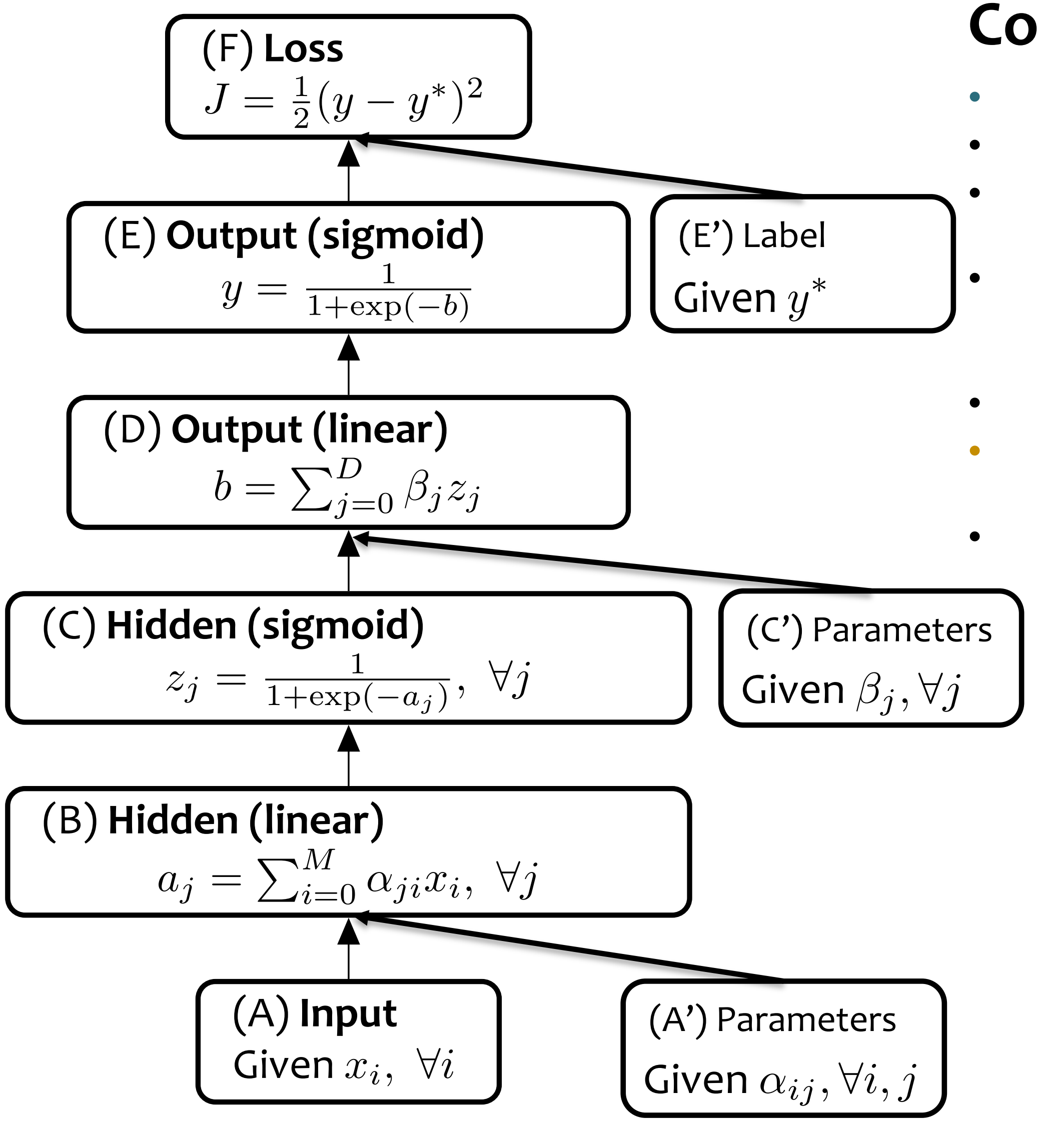
Ways of Drawing Neural Networks



Computation Graph

- The diagram represents an algorithm
- Nodes are **rectangles**
- One node per intermediate variable in the algorithm
- Node is labeled with the function that it computes (inside the box) and also the variable name (outside the box)
- *Edges are directed*
- Edges do not have labels (since they don't need them)
- For neural networks:
  - Each intercept term should appear as a node (if it's not folded in somewhere)
  - Each parameter should appear as a node
  - Each constant, e.g. a true label or a feature vector should appear in the graph
  - It's perfectly fine to include the loss

Ways of Drawing Neural Networks



(F) **Loss**
$J = \frac{1}{2}(y - y^*)^2$
(E) **Output (sigmoid)**
$y = \frac{1}{1+\exp(-b)}$
(E') Label
Given y^*
(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$
(C) **Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$
(C') Parameters
Given $\beta_j, \forall j$
(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$
(A) **Input**
Given $x_i, \ \forall i$
(A') Parameters
Given $\alpha_{ij}, \forall i, j$

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  - It's perfectly fine to include the loss

Important!

Some of these conventions are specific to 10-301/601. The literature abounds with varations on these conventions, but it's helpful to have *some* distinction nonetheless.

Summary

1. **Neural Networks…**
   - provide a way of learning features
   - are highly nonlinear prediction functions
   - (can be) a highly parallel network of logistic regression classifiers
   - discover useful hidden representations of the input
2. **Backpropagation…**
   - provides an efficient way to compute gradients
   - is a special case of reverse-mode automatic differentiation

Backprop Objectives

You should be able to…

- Differentiate between a neural network diagram and a computation graph
- Construct a computation graph for a function as specified by an algorithm
- Carry out the backpropagation on an arbitrary computation graph
- Construct a computation graph for a neural network, identifying all the given and intermediate quantities that are relevant
- Instantiate the backpropagation algorithm for a neural network
- Instantiate an optimization method (e.g. SGD) and a regularizer (e.g. L2) when the parameters of a model are comprised of several matrices corresponding to different layers of a neural network
- Apply the empirical risk minimization framework to learn a neural network
- Use the finite difference method to evaluate the gradient of a function
- Identify when the gradient of a function can be computed at all and when it can be computed efficiently
- Employ basic matrix calculus to compute vector/matrix/tensor derivatives.