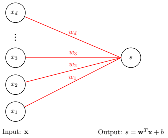
Lecture 3 - Back Propagation

DD2424

April 6, 2017

Classification functions we have encountered so far

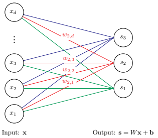
Linear with 1 output



Final decision:

$g(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$

Linear with multiple outputs

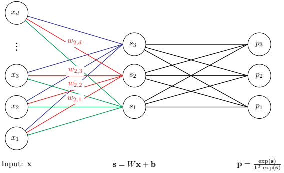


Final decision:

$g(\mathbf{x}) = \arg\max_j s_j$

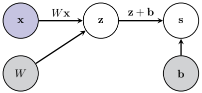
Classification functions we have encountered so far

Linear with multiple probabilistic outputs



Final decision: $g(\mathbf{x}) = \arg\max_j p_j$

Computational graph of the multiple linear function

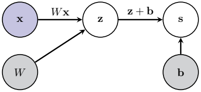


The computational graph:

- Represents order of computations.
- Displays the dependencies between the computed quantities.
- User input, parameters that have to be learnt.

Computational Graph helps automate gradient computations.

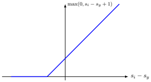
How do we learn $W, \mathbf{b}$?



- Assume have labelled training data $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$
- Set $W, \mathbf{b}$ so they correctly & robustly predict labels of the $\mathbf{x}_i$'s
- Need then to
  1. Measure the quality of the prediction's based on $W, \mathbf{b}$.
  2. Find the optimal $W, \mathbf{b}$ relative to the quality measure on the training data.

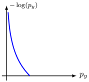
Quality measures a.k.a. loss functions we've encountered

Multi-class SVM loss



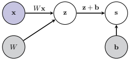
$$l_{\text{SVM}}(\mathbf{s}, y) = \sum_{\substack{j=1\\ j\neq y}}^{C} \max(0, s_j - s_y + 1)$$

Cross-entropy loss



$$l_{\text{c-e}}(\mathbf{p}, y) = -\log(p_y)$$

Classification function



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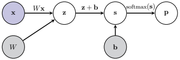
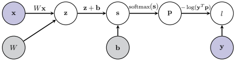


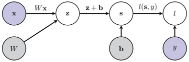
Computational graph of the complete loss function

- Linear scoring function + SOFTMAX + cross-entropy loss

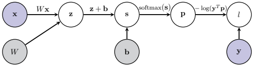


where $\mathbf{y}$ is the 1-hot response vector induced by the label y.

- Linear scoring function + multi-class SVM loss



How do we learn $W, \mathbf{b}$?



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- Set $W, \mathbf{b}$ so they correctly & robustly predict labels of the $\mathbf{x}_i$'s
- Need then to
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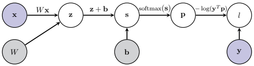
How do we learn $W, \mathbf{b}$?



- Let l be the loss function defined by the computational graph.
- Find $W, \mathbf{b}$ by optimizing

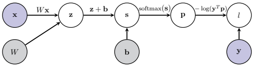
$$\arg\max_{W,\mathbf{b}} \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} l(\mathbf{x}, y, W, \mathbf{b})$$

- Solve using a variant of **mini-batch gradient descent**

$\Longrightarrow$ need to efficiently compute the gradient vectors

$$\nabla_W l(\mathbf{x}, y, W, \mathbf{b})|_{(\mathbf{x},y)\in\mathcal{D}} \quad \text{and} \quad \nabla_{\mathbf{b}} l(\mathbf{x}, y, W, \mathbf{b})|_{(\mathbf{x},y)\in\mathcal{D}}$$

How do we compute these gradients?



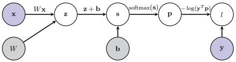
- Let l be the complete loss function defined by the computational graph.
- How do we efficiently compute the gradient vectors

$$\nabla_W l(\mathbf{x}, y, W, \mathbf{b})|_{(\mathbf{x},y)\in\mathcal{D}} \quad \text{and} \quad \nabla_{\mathbf{b}} l(\mathbf{x}, y, W, \mathbf{b})|_{(\mathbf{x},y)\in\mathcal{D}}?$$

- Answer: Back Propagation

Today's lecture: Gradient computations in neural networks

- For our learning approach need to be able to compute gradients efficiently.
- BackProp is algorithm for achieving given the form of many of our classifiers and loss functions.



- BackProp relies on the **chain rule** applied to the **composition of functions**.
- Example: the composition of functions

$$l(\mathbf{x}, y, W, \mathbf{b}) = -\log(\mathbf{y}^T \text{softmax}(W\mathbf{x} + \mathbf{b}))$$

linear classifier then **SOFTMAX** then **cross-entropy loss**

Chain Rule for functions with a scalar input and a scalar output

Differentiation of the composition of functions

- Have two functions $g : \mathbb{R} \to \mathbb{R}$ and $f : \mathbb{R} \to \mathbb{R}$.
- Define $h : \mathbb{R} \to \mathbb{R}$ as the composition of f and g:

$$h(x) = (f \circ g)(x) = f(g(x))$$

- How do we compute

$$\frac{dh(x)}{dx} \; ?$$

- Use the chain rule.

The Chain Rule

- Have functions $f, g : \mathbb{R} \to \mathbb{R}$ and define $h : \mathbb{R} \to \mathbb{R}$ as

$$h(x) = (f \circ g)(x) = f(g(x))$$

- Derivative of h w.r.t. x is given by the Chain Rule.
- **Chain Rule**

$$\frac{dh(x)}{dx} = \frac{df(y)}{dy}\frac{dg(x)}{dx} \quad \text{where } y = g(x)$$

Example of the Chain Rule in action

- Have

$$g(x) = x^2, \qquad f(x) = \sin(x)$$

- One composition of these two functions is

$$h(x) = f(g(x)) = \sin(x^2)$$

- According to the **chain rule**

$$\begin{aligned}\frac{dh(x)}{dx} &= \frac{df(y)}{dy}\frac{dg(x)}{dx} && \leftarrow \text{where } y = x^2\\ &= \frac{d\sin(y)}{dy}\frac{dx^2}{dx}\\ &= \cos(y)\,2x\\ &= 2x\cos(x^2) && \leftarrow \text{plug in } y = x^2\end{aligned}$$

The composition of n functions

- Have functions $f_1, \ldots, f_n : \mathbb{R} \to \mathbb{R}$
- Define function $h : \mathbb{R} \to \mathbb{R}$ as the composition of f_j's

$$h(x) = (f_n \circ f_{n-1} \circ \cdots \circ f_1)(x) = f_n(f_{n-1}(\cdots(f_1(x))\cdots)$$

- Can we compute the derivative

$$\frac{dh(x)}{dx} \quad ?$$

- Yes recursively apply the CHAIN RULE

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The Chain Rule for the composition of n functions

$$\boxed{h(x) = (f_n \circ f_{n-1} \circ \cdots \circ f_1)(x)}$$

- Define

$$g_j = f_n \circ f_{n-1} \circ \cdots \circ f_j$$

- Therefore $g_1 = h$, $g_n = f_n$ and

$$g_j = g_{j+1} \circ f_j \quad \text{for } j = 1, \ldots, n-1$$

- Let $y_j = f_j(y_{j-1})$ and $y_0 = x$ then

$$y_n = g_j(y_{j-1}) \quad \text{for } j = 1, \ldots, n$$

- Apply the **Chain Rule**:
  - For $j = 1, 2, 3, \ldots, n-1$

$$\frac{dy_n}{dy_{j-1}} = \frac{dg_j(y_{j-1})}{dy_{j-1}} = \frac{d\,(g_{j+1} \circ f_j)\,(y_{j-1})}{dy_{j-1}} = \frac{dg_{j+1}(y_j)}{dy_j}\frac{d\,f_j(y_{j-1})}{dy_{j-1}} = \frac{dy_n}{dy_j}\frac{dy_j}{dy_{j-1}}$$

The Chain Rule for the composition of n functions

Recursively applying this fact gives:

$$\begin{aligned}
\frac{dh(x)}{dx} &= \frac{dg_1(x)}{dx} && \leftarrow \text{Apply } h = g_1 \\
&= \frac{d(g_2 \circ f_1)(x)}{dx} && \leftarrow \text{Apply } g_1 = g_2 \circ f_1 \\
&= \frac{dg_2(y_1)}{dy_1}\frac{df_1(x)}{dx} && \leftarrow \text{Apply chain rule \& } y_1 = f_1(x) \\
&= \frac{d(g_3 \circ f_2)(y_1)}{dy_1}\frac{df_1(x)}{dx} && \leftarrow \text{Apply } g_2 = g_3 \circ f_2 \\
&= \frac{dg_3(y_2)}{dy_2}\frac{df_2(y_1)}{dy_1}\frac{df_1(x)}{dx} && \leftarrow \text{Apply chain rule \& } y_2 = f_2(y_1) \\
&\;\;\vdots \\
&= \frac{dg_n(y_{n-1})}{dy_{n-1}}\frac{df_{n-1}(y_{n-2})}{dy_{n-2}}\cdots\frac{df_2(y_1)}{dy_1}\frac{df_1(x)}{dx} \\
&= \frac{df_n(y_{n-1})}{dy_{n-1}}\frac{df_{n-1}(y_{n-2})}{dy_{n-2}}\cdots\frac{df_2(y_1)}{dy_1}\frac{df_1(x)}{dx} && \leftarrow \text{Apply } g_n = f_n
\end{aligned}$$

where $y_j = (f_j \circ f_{j-1} \circ \cdots \circ f_1)(x) = f_j(y_{j-1})$.

Summary: Chain Rule for a composition of n functions

- Have $f_1, \ldots, f_n : \mathbb{R} \to \mathbb{R}$ and define h as their composition

$$h(x) = (f_n \circ f_{n-1} \circ \cdots \circ f_1)(x)$$

- Then

$$\begin{aligned}
\frac{dh(x)}{dx} &= \frac{df_n(y_{n-1})}{dy_{n-1}}\frac{df_{n-1}(y_{n-2})}{dy_{n-2}}\cdots\frac{df_2(y_1)}{dy_1}\frac{df_1(x)}{dx} \\
&= \frac{dy_n}{dy_{n-1}}\,\frac{dy_{n-1}}{dy_{n-2}}\cdots\frac{dy_2}{dy_1}\,\frac{dy_1}{dx}
\end{aligned}$$

where $y_j = (f_j \circ f_{j-1} \circ \cdots \circ f_1)(x) = f_j(y_{j-1})$.

- **Remember**: As $y_0 = x$ then for $j = n-1, n-2, \ldots, 0$

$$\frac{dy_n}{dy_j} = \frac{dy_n}{dy_{j+1}}\,\frac{dy_{j+1}}{dy_j}$$

Summary: Chain Rule for a composition of n functions

- Have $f_1, \ldots, f_n : \mathbb{R} \rightarrow \mathbb{R}$ and define h as their composition

$$h(x) = (f_n \circ f_{n-1} \circ \cdots \circ f_1)(x)$$

- Then

$$\frac{dh(x)}{dx} = \frac{df_n(y_{n-1})}{dy_{n-1}} \frac{df_{n-1}(y_{n-2})}{dy_{n-2}} \cdots \frac{df_2(y_1)}{dy_1} \frac{df_1(x)}{dx}$$
$$= \frac{dy_n}{dy_{n-1}} \frac{dy_{n-1}}{dy_{n-2}} \cdots \frac{dy_2}{dy_1} \frac{dy_1}{dx}$$

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Exploit structure to compute gradient

$$\frac{dh(x)}{dx} = \frac{dy_n}{dx} = \frac{dy_n}{dy_{n-1}} \frac{dy_{n-1}}{dy_{n-2}} \cdots \frac{dy_2}{dy_1} \frac{dy_1}{dx}$$

Computation of $\frac{dy_n}{dx}$ relies on:

- **Record keeping**: Compute and record values of the y_j's.
- **Iteratively aggregate** local gradients.
  For $j = n-1, n, \ldots, 1$
  - Compute local derivative: $\frac{df_{j+1}(y_j)}{dy_j} = \frac{dy_{j+1}}{dy_j}$
  - Aggregate:

$$\frac{dy_n}{dy_j} = \frac{dy_n}{dy_{j+1}} \frac{dy_{j+1}}{dy_j}$$

Remember $\frac{dy_n}{dy_{j+1}} = \frac{dy_n}{dy_{n-1}} \frac{dy_{n-1}}{dy_{n-2}} \cdots \frac{dy_{j+2}}{dy_{j+1}}$

This is Backprop algorithm given a chain dependency between the y_j's.

Exploit structure to compute gradient

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This is Backprop algorithm given a chain dependency between the y_j's.

Compute gradient of h at a point x^*

$$h(x) = (f_n \circ f_{n-1} \circ \cdots \circ f_1)(x)$$

- Have a value for $x = x^*$
- Want to (efficiently) compute

$$\left.\frac{dh(x)}{dx}\right|_{x=x^*}$$

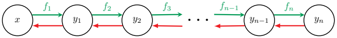
- Use the **Back-Propagation** algorithm.
- It consists of a Forward and Backward pass.

Back-Propagation for chains: Forward Pass

Evaluate $h(x^*)$ and keep track of the intermediary results

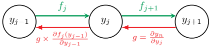
- Compute $y_1^* = f_1(x^*)$.
- for $j = 2, 3, \ldots, n$
$$y_j^* = f_j(y_{j-1}^*)$$
- Keep a record of $y_1^*, \ldots, y_n^*$.

Back-Propagation for chains: Backward Pass



Compute local f_j gradients and aggregate:

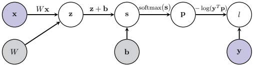
- Set $g = 1$.
- for $j = n, n-1, \ldots, 2$
$$g = g \times \left. \frac{df_j(y_{j-1})}{dy_{j-1}} \right|_{y_{j-1} = y_{j-1}^*}$$



Note: $g = \left. \frac{dy_n}{dy_{j-1}} \right|_{y_{j-1} = y_{j-1}^*}$

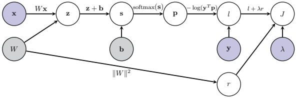
- Then $\left. \frac{dh(x)}{dx} \right|_{x = x^*} = g \times \left. \frac{df_1(x)}{dx} \right|_{x = x^*}$

Problem 1: But what if I don't have a chain?



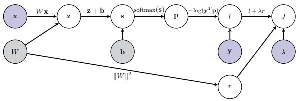
- This computational graph is **not a chain**.
- Some nodes have multiple parents.
- The function represented by graph is
$$l(\mathbf{x}, \mathbf{y}, W, \mathbf{b}) = -\log(\mathbf{y}^T \text{Softmax}(W\mathbf{x} + \mathbf{b}))$$

Problem 1a: And when a regularization term is added..



- This computational graph is **not a chain**.
- Some nodes have **multiple parents** and others **multiple children**.
- The function represented by graph is
$$J(\mathbf{x}, \mathbf{y}, W, \mathbf{b}, \lambda) = -\log(\mathbf{y}^T \text{Softmax}(W\mathbf{x} + \mathbf{b})) + \lambda \sum_{i,j} W_{i,j}^2$$
- How is the back-propagation algorithm defined in these cases?

Problem 1a: And when a regularization term is added..



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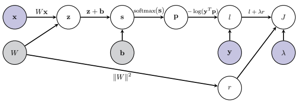
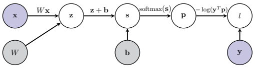
Problem 2: Don't have scalar inputs and outputs



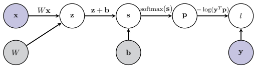
- The function represented by graph:
$$J(\mathbf{x}, \mathbf{y}, W, \mathbf{b}, \lambda) = -\log(\mathbf{y}^T \text{Softmax}(W\mathbf{x} + \mathbf{b})) + \lambda \sum_{i,j} W_{i,j}^2$$
- Nearly all of the inputs and intermediary outputs are **vectors** or **matrices**.
- How are the derivatives defined in this case?

Issues we need to sort out



- Back-propagation when the computational graph is **not a chain**.
- Derivative computations when the inputs and outputs are not scalars.
- Will address these issues now. First the derivatives of vectors.

Issues we need to sort out



- Back-propagation when the computational graph is **not a chain**.
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Chain Rule for functions with vector inputs and vector outputs

Chain Rule for vector input and output

- Have two functions $g : \mathbb{R}^d \to \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}^c$.
- Define $h : \mathbb{R}^d \to \mathbb{R}^c$ as the composition of f and g:

$$h(\mathbf{x}) = (f \circ g)(\mathbf{x}) = f(g(\mathbf{x}))$$

- Consider

$$\frac{\partial h(\mathbf{x})}{\partial \mathbf{x}}$$

- How is it defined and computed?
- What's the chain rule for vector valued functions?

Chain Rule for vector input and output

- Let $\mathbf{y} = h(\mathbf{x})$ where each $h : \mathbb{R}^d \to \mathbb{R}^c$ then

$$\frac{\partial h(\mathbf{x})}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_d} \\ \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_2}{\partial x_d} \\ \vdots & \vdots & \vdots \\ \frac{\partial y_c}{\partial x_1} & \cdots & \frac{\partial y_c}{\partial x_d} \end{pmatrix} \quad \leftarrow \text{this is a Jacobian matrix}$$

  and is a matrix of size $c \times d$.

- **Chain Rule** says if $h = f \circ g$ ($g : \mathbb{R}^d \to \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}^c$) then

$$\frac{\partial h(\mathbf{x})}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{x}}$$

  where $\mathbf{z} = g(\mathbf{x})$ and $\mathbf{y} = f(\mathbf{z})$.

- Both $\frac{\partial \mathbf{y}}{\partial \mathbf{z}}$ $(c \times m)$ and $\frac{\partial \mathbf{z}}{\partial \mathbf{x}}$ $(m \times d)$ defined slly to $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$.

Chain Rule for vector input and scalar output

The cost functions we will examine usually have a scalar output

- Let $\mathbf{x} \in \mathbb{R}^d$, $f : \mathbb{R}^d \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}$

$$\mathbf{z} = f(\mathbf{x})$$
$$s = g(\mathbf{z})$$

- The **Chain Rule** says gradient of output w.r.t. input

$$\frac{\partial s}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial s}{\partial x_1} & \cdots & \frac{\partial s}{\partial x_d} \end{pmatrix}$$

  is given by a gradient times a Jacobian:

$$\frac{\partial s}{\partial \mathbf{x}} = \underbrace{\frac{\partial s}{\partial \mathbf{z}}}_{1 \times m} \underbrace{\frac{\partial \mathbf{z}}{\partial \mathbf{x}}}_{m \times d}$$

  where

$$\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_d} \\ \frac{\partial z_2}{\partial x_1} & \cdots & \frac{\partial z_2}{\partial x_d} \\ \vdots & \vdots & \vdots \\ \frac{\partial z_m}{\partial x_1} & \cdots & \frac{\partial z_m}{\partial x_d} \end{pmatrix}$$

Two intermediary vector inputs and scalar output

- $f_1 : \mathbb{R}^d \to \mathbb{R}^{m_1}$, $f_2 : \mathbb{R}^d \to \mathbb{R}^{m_2}$ and $g : \mathbb{R}^n \to \mathbb{R}$ $(n = m_1 + m_2)$

$$\mathbf{z}_1 = f_1(\mathbf{x}), \qquad \mathbf{z}_2 = f_2(\mathbf{x})$$

$$s = g(\mathbf{z}_1, \mathbf{z}_2) = g(\mathbf{v}) \qquad \text{where } \mathbf{v} = \begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \end{pmatrix}.$$

- **Chain Rule** says gradient of the output w.r.t. the input

$$\frac{\partial s}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial s}{\partial x_1} & \cdots & \frac{\partial s}{\partial x_d} \end{pmatrix}$$

is given by:

$$\frac{\partial s}{\partial \mathbf{x}} = \underbrace{\frac{\partial s}{\partial \mathbf{v}}}_{1 \times n} \underbrace{\frac{\partial \mathbf{v}}{\partial \mathbf{x}}}_{n \times d}$$

But

$$\frac{\partial s}{\partial \mathbf{v}} = \begin{pmatrix} \frac{\partial s}{\partial \mathbf{z}_1} & \frac{\partial s}{\partial \mathbf{z}_2} \end{pmatrix} \quad \text{and} \quad \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial \mathbf{z}_1}{\partial \mathbf{x}} \\ \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}} \end{pmatrix}$$

$\Longrightarrow$

$$\frac{\partial s}{\partial \mathbf{x}} = \frac{\partial s}{\partial \mathbf{v}} \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \underbrace{\frac{\partial s}{\partial \mathbf{z}_1}}_{1 \times m_1} \underbrace{\frac{\partial \mathbf{z}_1}{\partial \mathbf{x}}}_{m_1 \times d} + \underbrace{\frac{\partial s}{\partial \mathbf{z}_2}}_{1 \times m_2} \underbrace{\frac{\partial \mathbf{z}_2}{\partial \mathbf{x}}}_{m_2 \times d}$$

More generally

- $f_i : \mathbb{R}^d \to \mathbb{R}^{m_i}$ for $i = 1, \ldots, t$ and $g : \mathbb{R}^n \to \mathbb{R}$ $(n = m_1 + \cdots + m_t)$

$$\mathbf{z}_i = f_i(\mathbf{x}), \qquad \text{for } i = 1, \ldots, t$$

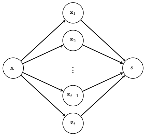
$$s = g(\mathbf{z}_1, \ldots, \mathbf{z}_n)$$

- Consequence of the **Chain Rule**

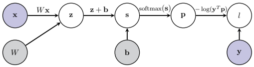
$$\frac{\partial s}{\partial \mathbf{x}} = \sum_{i=1}^{t} \frac{\partial s}{\partial \mathbf{z}_i} \frac{\partial \mathbf{z}_i}{\partial \mathbf{x}}$$

- Computational graph interpretation. Let $\mathcal{C}_{\mathbf{x}}$ be the children nodes of $\mathbf{x}$ then

$$\frac{\partial s}{\partial \mathbf{x}} = \sum_{\mathbf{z} \in \mathcal{C}_{\mathbf{x}}} \frac{\partial s}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{x}}$$



Issues we need to sort out



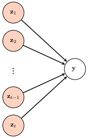
- Back-propagation when the computational graph is **not a chain**.
- Derivative computations when the inputs and outputs are not scalars. ✓
- Will now describe Back-prop for non-chains.

Back-propagation for non-chain computational graphs

Results that we need

- Have node $\mathbf{y}$.
- Denote the set of $\mathbf{y}$'s parent nodes by $\mathcal{P}_\mathbf{y}$ and their values by

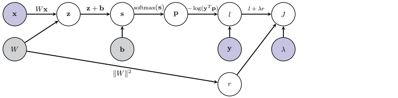
$$V_{\mathcal{P}_\mathbf{y}} = \{\mathbf{z}.\text{value} \mid \mathbf{z} \in \mathcal{P}_\mathbf{y}\}$$



- Given $V_{\mathcal{P}_\mathbf{y}}$ can now apply the function $f_\mathbf{z}$

$$\mathbf{y}.\text{value} = f_\mathbf{y}(V_{\mathcal{P}_\mathbf{y}})$$

Results that we need but already know



- Consider node W in the above graph. Its children are $\{\mathbf{z}, r\}$. Applying the chain rule

$$\frac{\partial J}{\partial W} = \frac{\partial J}{\partial r}\frac{\partial r}{\partial W} + \frac{\partial J}{\partial \mathbf{z}}\frac{\partial \mathbf{z}}{\partial W}$$

- In general for node $\mathbf{c}$ with children specified by $\mathcal{C}_\mathbf{c}$:

$$\frac{\partial J}{\partial \mathbf{c}} = \sum_{\mathbf{u}\in\mathcal{C}_\mathbf{c}} \frac{\partial J}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{c}}$$

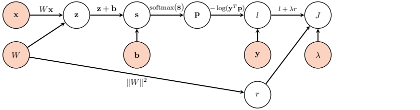
Pseudo-Code for the Generic Forward Pass

```
procedure EVAULATEGRAPHFN(G)                         ▷ G is the computational graph
    S = GetStartNodes(G)          ▷ a start node has no parent and its value is already set
    for s ∈ S do
        ComputeBranch(s, G)
    end for
end procedure

procedure COMPUTEBRANCH(s, G)                        ▷ recursive fn evaluating nodes
    C_s = GetChildren(s, G)
    for each n ∈ C_s do                              ▷ Try to evaluate each children node
        if !n.computed then                          ▷ Unless child is already computed
            P_n = GetParents(n, G)
            if CheckAllNodesComputed(P_n) then ▷ Or not all parents of children are computed
                f_n = GetNodeFn(n)
                n.value = f_n(P_n)
                n.computed = true
                ComputeBranch(n, G)
            end if
        end if
    end for
end procedure
```

Generic Forward Pass

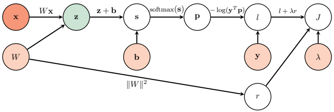
Identify Start Nodes




```
procedure EVAULATEGRAPHFN(G)    ▷ G is the computational graph
    S = GetStartNodes(G)
    for s ∈ S do
        ComputeBranch(s, G)
    end for
end procedure

procedure COMPUTEBRANCH(s, G)
    C_s = GetChildren(s, G)
    for each n ∈ C_s do
        if !n.computed then
            P_n = GetParents(n, G)
            if CheckAllNodesComputed(P_n) then
                f_n = GetNodeFn(n)
                n.value = f_n(P_n)
                n.computed = true
                ComputeBranch(n, G)
            end if
        end if
    end for
end procedure
```

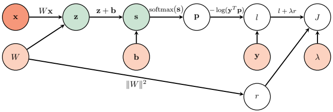
Order in which nodes are evaluated



procedure EVAULATEGRAPHFN(G) ▷ G is the computational graph
$\mathcal{S}$ = GetStartNodes(G)
for s $\in \mathcal{S}$ **do**
ComputeBranch(s, G)
end for
end procedure

procedure COMPUTEBRANCH($\mathbf{s}$, G)
$\mathcal{P}_{\mathbf{s}}$ = GetParents(s, G)
for each $\mathbf{n} \in \mathcal{P}_{\mathbf{s}}$ **do**
if !$\mathbf{n}$.computed **then**
$\mathcal{C}_{\mathbf{n}}$ = GetChildren($\mathbf{n}$, G)
if CheckAllNodesComputed($\mathcal{C}_{\mathbf{n}}$) **then**
$f_{\mathbf{n}}$ = GetNodeFn($\mathbf{n}$)
$\mathbf{n}$.value = $f_{\mathbf{n}}(\mathcal{C}_{\mathbf{n}})$
$\mathbf{n}$.computed = true
ComputeBranch($\mathbf{n}$, G)
end if
end if
end for
end procedure

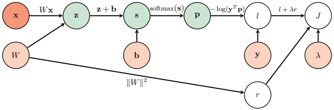
Order in which nodes are evaluated



procedure EVAULATEGRAPHFN(G) ▷ G is the computational graph
$\mathcal{S}$ = GetStartNodes(G)
for s $\in \mathcal{S}$ **do**
ComputeBranch(s, G)
end for
end procedure

procedure COMPUTEBRANCH($\mathbf{s}$, G)
$\mathcal{P}_{\mathbf{s}}$ = GetParents(s, G)
for each $\mathbf{n} \in \mathcal{P}_{\mathbf{s}}$ **do**
if !$\mathbf{n}$.computed **then**
$\mathcal{C}_{\mathbf{n}}$ = GetChildren($\mathbf{n}$, G)
if CheckAllNodesComputed($\mathcal{C}_{\mathbf{n}}$) **then**
$f_{\mathbf{n}}$ = GetNodeFn($\mathbf{n}$)
$\mathbf{n}$.value = $f_{\mathbf{n}}(\mathcal{C}_{\mathbf{n}})$
$\mathbf{n}$.computed = true
ComputeBranch($\mathbf{n}$, G)
end if
end if
end for
end procedure

Order in which nodes are evaluated



procedure EVAULATEGRAPHFN(G) ▷ G is the computational graph
$\mathcal{S}$ = GetStartNodes(G)
for s $\in \mathcal{S}$ **do**
ComputeBranch(s, G)
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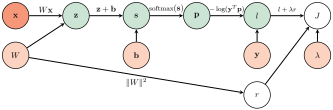
procedure COMPUTEBRANCH($\mathbf{s}$, G)
$\mathcal{P}_{\mathbf{s}}$ = GetParents(s, G)
for each $\mathbf{n} \in \mathcal{P}_{\mathbf{s}}$ **do**
if !$\mathbf{n}$.computed **then**
$\mathcal{C}_{\mathbf{n}}$ = GetChildren($\mathbf{n}$, G)
if CheckAllNodesComputed($\mathcal{C}_{\mathbf{n}}$) **then**
$f_{\mathbf{n}}$ = GetNodeFn($\mathbf{n}$)
$\mathbf{n}$.value = $f_{\mathbf{n}}(\mathcal{C}_{\mathbf{n}})$
$\mathbf{n}$.computed = true
ComputeBranch($\mathbf{n}$, G)
end if
end if
end for
end procedure

Order in which nodes are evaluated

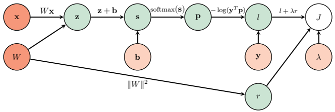


procedure EVAULATEGRAPHFN(G) ▷ G is the computational graph
$\mathcal{S}$ = GetStartNodes(G)
for s $\in \mathcal{S}$ **do**
ComputeBranch(s, G)
end for
end procedure

procedure COMPUTEBRANCH($\mathbf{s}$, G)
$\mathcal{P}_{\mathbf{s}}$ = GetParents(s, G)
for each $\mathbf{n} \in \mathcal{P}_{\mathbf{s}}$ **do**
if !$\mathbf{n}$.computed **then**
$\mathcal{C}_{\mathbf{n}}$ = GetChildren($\mathbf{n}$, G)
if CheckAllNodesComputed($\mathcal{C}_{\mathbf{n}}$) **then**
$f_{\mathbf{n}}$ = GetNodeFn($\mathbf{n}$)
$\mathbf{n}$.value = $f_{\mathbf{n}}(\mathcal{C}_{\mathbf{n}})$
$\mathbf{n}$.computed = true
ComputeBranch($\mathbf{n}$, G)
end if
end if
end for
end procedure

Generic Forward Pass

Order in which nodes are evaluated

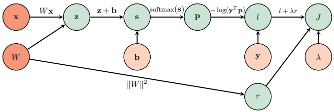



```
procedure EvaulateGraphFn(G)          ▷ G is the computational graph
    $\mathcal{S}$ = GetStartNodes(G)
    for s ∈ $\mathcal{S}$ do
        ComputeBranch(s, G)
    end for
end procedure
```

```
procedure ComputeBranch(s, G)
    $\mathcal{P}_\mathbf{s}$ = GetParents(s, G)
    for each n ∈ $\mathcal{P}_\mathbf{s}$ do
        if !n.computed then
            $\mathcal{C}_\mathbf{n}$ = GetChildren(n, G)
            if CheckAllNodesComputed($\mathcal{C}_\mathbf{n}$) then
                $f_\mathbf{n}$ = GetNodeFn(n)
                n.value = $f_\mathbf{n}(\mathcal{C}_\mathbf{n})$
                n.computed = true
                ComputeBranch(n, G)
            end if
        end if
    end for
end procedure
```

Generic Forward Pass

Order in which nodes are evaluated




```
procedure EvaulateGraphFn(G)          ▷ G is the computational graph
    $\mathcal{S}$ = GetStartNodes(G)
    for s ∈ $\mathcal{S}$ do
        ComputeBranch(s, G)
    end for
end procedure
```

```
procedure ComputeBranch(s, G)
    $\mathcal{P}_\mathbf{s}$ = GetParents(s, G)
    for each n ∈ $\mathcal{P}_\mathbf{s}$ do
        if !n.computed then
            $\mathcal{C}_\mathbf{n}$ = GetChildren(n, G)
            if CheckAllNodesComputed($\mathcal{C}_\mathbf{n}$) then
                $f_\mathbf{n}$ = GetNodeFn(n)
                n.value = $f_\mathbf{n}(\mathcal{C}_\mathbf{n})$
                n.computed = true
                ComputeBranch(n, G)
            end if
        end if
    end for
end procedure
```

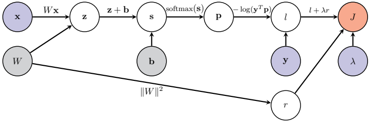

Pseudo-Code for the Generic Backward Pass

```
procedure PerformBackPass(G)
    $J$ = GetResultNode(G)                    ▷ node with the value of cost function
    BackOp($J$, G)                            ▷ Start the Backward-pass
end procedure

procedure BackOp(s, G)
    $\mathcal{C}_\mathbf{s}$ = GetChildren(s, G)
    if $\mathcal{C}_\mathbf{s} = \emptyset$ then                 ▷ At the result node
        s.Grad = 1
    end if
    if AllGradientsComputed($\mathcal{C}_\mathbf{s}$) then    ▷ Have computed all $\frac{\partial J}{\partial \mathbf{c}}$ where $\mathbf{c} \in \mathcal{C}_\mathbf{s}$
        s.Grad = 0
        for each c ∈ $\mathcal{C}_\mathbf{s}$ do
            s.Grad += c.Grad * c.s.Jacobian     ▷ $\frac{\partial J}{\partial \mathbf{s}}$ += $\frac{\partial J}{\partial \mathbf{c}} \frac{\partial \mathbf{c}}{\partial \mathbf{s}}$
        end for
        s.GradComputed = true
    end if
    for each p ∈ $\mathcal{P}_\mathbf{s}$ do           ▷ Compute the Jacobian of $f_\mathbf{s}$ w.r.t. each parent node
        s.p.Jacobian = $\frac{\partial f_\mathbf{p}(\mathcal{P}_\mathbf{s})}{\partial \mathbf{p}}$        ▷ $\frac{\partial f_\mathbf{s}(\mathcal{P}_\mathbf{s})}{\partial \mathbf{p}} = \frac{\partial \mathbf{s}}{\partial \mathbf{p}}$
        BackOp(p, G)
    end for
end procedure
```

Generic Backward Pass: Order of computations

Identify Result Node

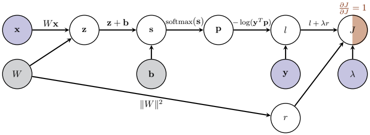



```
procedure PerformBackPass(G)
    $J$ = GetResultNode(G)     ▷ node with the value of cost function
    BackOp($J$, G)             ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    $\mathcal{C}_\mathbf{s}$ = GetChildren(s, G)
    if $\mathcal{C}_\mathbf{s} = \emptyset$ then                  ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed($\mathcal{C}_\mathbf{s}$) then   ▷ All $\frac{\partial J}{\partial \mathbf{c}}$ computed where $\mathbf{c} \in \mathcal{C}_\mathbf{s}$
            s.Grad = 0
            for each c ∈ $\mathcal{C}_\mathbf{s}$ do
                s.Grad += c.Grad * c.s.Jacobian     ▷ $\frac{\partial J}{\partial \mathbf{s}}$ += $\frac{\partial J}{\partial \mathbf{c}} \frac{\partial \mathbf{c}}{\partial \mathbf{s}}$
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ $\mathcal{P}_\mathbf{s}$ do     ▷ Compute Jacobian of $f_\mathbf{s}$ w.r.t. each parent node
        s.p.Jacobian = $\frac{\partial f_\mathbf{s}(\mathcal{P}_\mathbf{s})}{\partial \mathbf{p}}$     ▷ $\frac{\partial f_\mathbf{s}(\mathcal{P}_\mathbf{s})}{\partial \mathbf{p}} = \frac{\partial \mathbf{s}}{\partial \mathbf{p}}$
        BackOp(p, G)
    end for
end procedure
```

Generic Backward Pass: Order of computations

Compute Gradient of current node

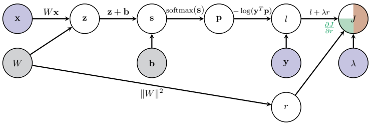



```
procedure PerformBackPass(G)
    J = GetResultNode(G)     ▷ node with the value of cost function
    BackOp(J, G)             ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                   ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed(C_s) then             ▷ All ∂J/∂c computed where c ∈ C_s
            s.Grad = 0
            for each c ∈ C_s do
                s.Grad += c.Grad * c.s.Jacobian       ▷ ∂J/∂s += ∂J/∂c ∂c/∂s
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ P_s do                               ▷ Compute Jacobian of f_s w.r.t. each parent node
        s.p.Jacobian = ∂f_s(P_s)/∂p                   ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```


Generic Backward Pass: Order of computations

Compute Jacobian of current node w.r.t. its child

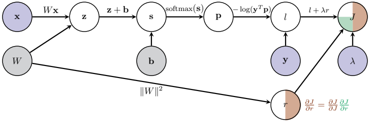



```
procedure PerformBackPass(G)
    J = GetResultNode(G)     ▷ node with the value of cost function
    BackOp(J, G)             ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                   ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed(C_s) then             ▷ All ∂J/∂c computed where c ∈ C_s
            s.Grad = 0
            for each c ∈ C_s do
                s.Grad += c.Grad * c.s.Jacobian       ▷ ∂J/∂s += ∂J/∂c ∂c/∂s
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ P_s do                               ▷ Compute Jacobian of f_s w.r.t. each parent node
        s.p.Jacobian = ∂f_s(P_s)/∂p                   ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```


Generic Backward Pass: Order of computations

Compute Gradient of current node

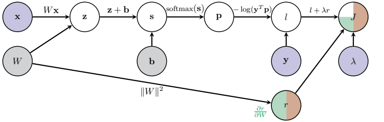



```
procedure PerformBackPass(G)
    J = GetResultNode(G)     ▷ node with the value of cost function
    BackOp(J, G)             ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                   ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed(C_s) then             ▷ All ∂J/∂c computed where c ∈ C_s
            s.Grad = 0
            for each c ∈ C_s do
                s.Grad += c.Grad * c.s.Jacobian       ▷ ∂J/∂s += ∂J/∂c ∂c/∂s
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ P_s do                               ▷ Compute Jacobian of f_s w.r.t. each parent node
        s.p.Jacobian = ∂f_s(P_s)/∂p                   ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```


Generic Backward Pass: Order of computations

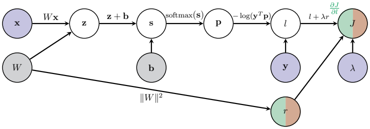
Compute Jacobian of current node w.r.t. its child




```
procedure PerformBackPass(G)
    J = GetResultNode(G)     ▷ node with the value of cost function
    BackOp(J, G)             ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                   ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed(C_s) then             ▷ All ∂J/∂c computed where c ∈ C_s
            s.Grad = 0
            for each c ∈ C_s do
                s.Grad += c.Grad * c.s.Jacobian       ▷ ∂J/∂s += ∂J/∂c ∂c/∂s
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ P_s do                               ▷ Compute Jacobian of f_s w.r.t. each parent node
        s.p.Jacobian = ∂f_s(P_s)/∂p                   ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```

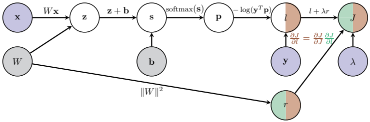
Compute Jacobian of current node w.r.t. its child




```
procedure PerformBackPass(G)
    J = GetResultNode(G)        ▷ node with the value of cost function
    BackOp(J, G)                ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                         ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed(C_s) then      ▷ All ∂J/∂c computed where c ∈ C_s
            s.Grad = 0
            for each c ∈ C_s do
                s.Grad += c.Grad * c.s.Jacobian           ▷ ∂J/∂s += ∂J/∂c ∂c/∂s
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ P_s do        ▷ Compute Jacobian of f_s w.r.t. each parent node
        s.p.Jacobian = ∂f_s(P_s)/∂p                      ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```

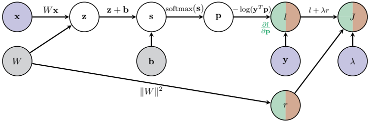

Compute Gradient of current node




```
procedure PerformBackPass(G)
    J = GetResultNode(G)        ▷ node with the value of cost function
    BackOp(J, G)                ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                         ▷ At the result node
        s.Grad = 1
    else
        if AllGradientsComputed(C_s) then      ▷ All ∂J/∂c computed where c ∈ C_s
            s.Grad = 0
            for each c ∈ C_s do
                s.Grad += c.Grad * c.s.Jacobian           ▷ ∂J/∂s += ∂J/∂c ∂c/∂s
            end for
            s.GradComputed = true
        end if
    end if
    for each p ∈ P_s do        ▷ Compute Jacobian of f_s w.r.t. each parent node
        s.p.Jacobian = ∂f_s(P_s)/∂p                      ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```


Compute Jacobian of current node w.r.t. its child




```
procedure PerformBackPass(G)
    J = GetResultNode(G)        ▷ node with the value of cost function
    BackOp(J, G)                ▷ Start the Backward-pass
end procedure
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```
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            end for
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        end if
    end if
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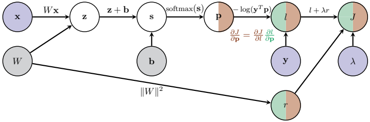
        s.p.Jacobian = ∂f_s(P_s)/∂p                      ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```


Compute Gradient of current node




```
procedure PerformBackPass(G)
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    BackOp(J, G)                ▷ Start the Backward-pass
end procedure
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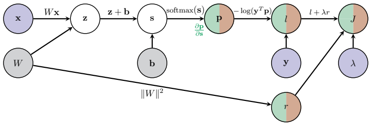
        BackOp(p, G)
    end for
end procedure
```

Compute Jacobian of current node w.r.t. its child




```
procedure PerformBackPass(G)
    J = GetResultNode(G)        ▷ node with the value of cost function
    BackOp(J, G)                ▷ Start the Backward-pass
end procedure
```

```
procedure BackOp(s, G)
    C_s = GetChildren(s, G)
    if C_s = ∅ then                                   ▷ At the result node
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    else
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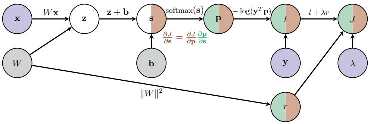
        s.p.Jacobian = ∂f_s(P_s)/∂p                   ▷ ∂f_s(P_s)/∂p = ∂s/∂p
        BackOp(p, G)
    end for
end procedure
```


Compute Gradient of current node

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    J = GetResultNode(G)        ▷ node with the value of cost function
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end procedure
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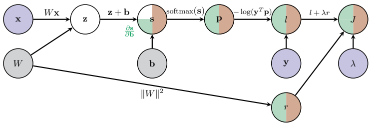
        BackOp(p, G)
    end for
end procedure
```


Compute Jacobian of current node w.r.t. its child




```
procedure PerformBackPass(G)
    J = GetResultNode(G)        ▷ node with the value of cost function
    BackOp(J, G)                ▷ Start the Backward-pass
end procedure
```

```
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    for each p ∈ P_s do                               ▷ Compute Jacobian of f_s w.r.t. each parent node
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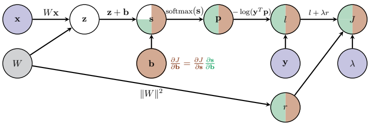
        BackOp(p, G)
    end for
end procedure
```


Compute Gradient of current node

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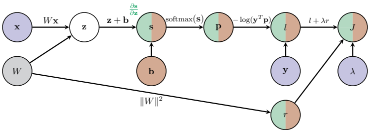
    end for
end procedure
```

Compute Jacobian of current node w.r.t. its child



procedure PerformBackPass(G)
  J = GetResultNode(G) ▷ node with the value of cost function
  BackOp(J, G) ▷ Start the Backward-pass
end procedure

procedure BackOp($\mathbf{s}$, G)
  $\mathcal{C}_{\mathbf{s}}$ = GetChildren($\mathbf{s}$, G)
  if $\mathcal{C}_{\mathbf{s}} = \emptyset$ **then** ▷ At the result node
    $\mathbf{s}$.Grad = 1
  else
    if AllGradientsComputed($\mathcal{C}_{\mathbf{s}}$) **then** ▷ All $\frac{\partial J}{\partial \mathbf{c}}$ computed where $\mathbf{c} \in \mathcal{C}_{\mathbf{s}}$
      $\mathbf{s}$.Grad = $\mathbf{0}$
      for each $\mathbf{c} \in \mathcal{C}_{\mathbf{s}}$ **do**
        $\mathbf{s}$.Grad += $\mathbf{c}$.Grad * $\mathbf{c}$.$\mathbf{s}$.Jacobian ▷ $\frac{\partial J}{\partial \mathbf{s}}$ += $\frac{\partial J}{\partial \mathbf{c}}\frac{\partial \mathbf{c}}{\partial \mathbf{s}}$
      end for
      $\mathbf{s}$.GradComputed = true
    end if
  end if
  for each $\mathbf{p} \in \mathcal{P}_{\mathbf{s}}$ **do** ▷ Compute Jacobian of $f_{\mathbf{s}}$ w.r.t. each parent node
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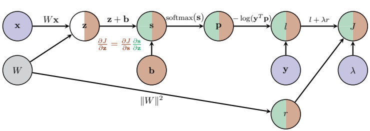
    BackOp($\mathbf{p}$, G)
  end for
end procedure

Compute Gradient of current node



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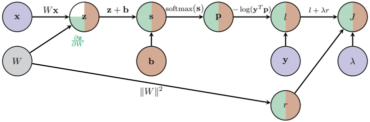
  end for
end procedure

Compute Jacobian of current node w.r.t. its child



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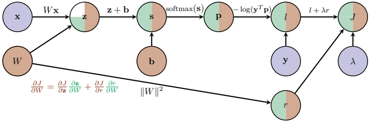
    BackOp($\mathbf{p}$, G)
  end for
end procedure

Compute Gradient of current node



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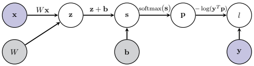
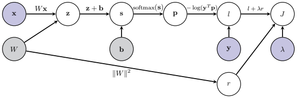
Issues we need to sort out



- Back-propagation when the computational graph is **not a chain**. ✓
- Derivative computations when the inputs and outputs are not scalars. ✓
- Let's now compute some gradients!

Example of the chain rule in action

Compute gradients for

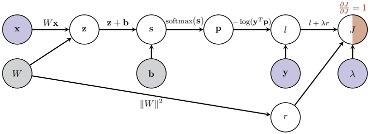


linear scoring function + SOFTMAX + cross-entropy loss + Regularization

- Assume the forward pass has been completed.
- $\Longrightarrow$ value for every node is known.

Generic Backward Pass: Gradient of current node

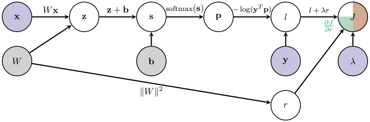
Compute Gradient of node J



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

Generic Backward Pass: Order of computations

Compute Jacobian of node J w.r.t. its child r

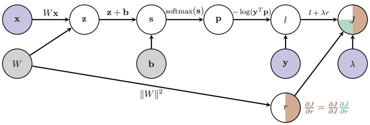


$$\boxed{J = l + \lambda r}$$

$$\frac{\partial J}{\partial r} = \lambda$$

Generic Backward Pass: Order of computations

Compute Gradient of node r

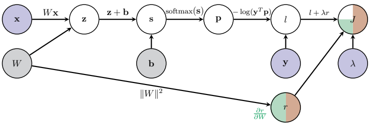


$$\boxed{J = l + \lambda r}$$

$$\frac{\partial J}{\partial r} = \frac{\partial J}{\partial J}\frac{\partial J}{\partial r} = \lambda$$

Generic Backward Pass: Order of computations

Compute Jacobian of node r w.r.t. its child W

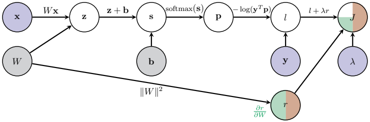


$$\boxed{r = \sum_{i,j} W_{ij}^2}$$

$$\frac{\partial r}{\partial W} = ?$$

Derivative of a scalar w.r.t. a matrix

Generic Backward Pass: Compute Jacobian



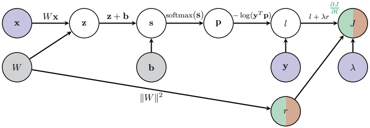
$$\boxed{r = \sum_{i,j} W_{ij}^2}$$

- Jacobian to compute: $\frac{\partial r}{\partial W} = \begin{pmatrix} \frac{\partial r}{\partial W_{11}} & \frac{\partial r}{\partial W_{12}} & \cdots & \cdots \frac{\partial r}{\partial W_{1d}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial r}{\partial W_{C1}} & \frac{\partial r}{\partial W_{C2}} & \cdots & \cdots \frac{\partial r}{\partial W_{Cd}} \end{pmatrix}$
- The individual derivatives: $\frac{\partial r}{\partial W_{ij}} = 2W_{ij}$
- Putting it together in matrix notation

$$\frac{\partial r}{\partial W} = 2W$$

Generic Backward Pass: Order of computations

Compute Jacobian of node J w.r.t. its child l

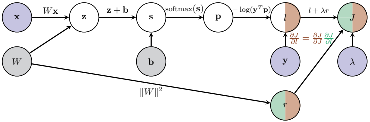


$$\boxed{J = l + \lambda r}$$

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

Generic Backward Pass: Order of computations

Compute Gradient of node l

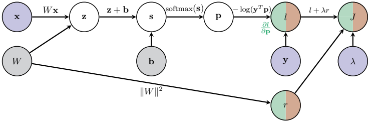


$$\boxed{J = l + \lambda r}$$

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

Generic Backward Pass: Order of computations

Compute Jacobian of node l w.r.t. its child $\mathbf{p}$



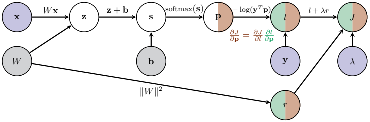
$$\boxed{l = -\log(\mathbf{y}^T\mathbf{p})}$$

- The Jacobian we want to compute: $\frac{\partial l}{\partial \mathbf{p}} = \left(\frac{\partial l}{\partial p_1}, \quad \frac{\partial l}{\partial p_2}, \quad \cdots \quad, \frac{\partial l}{\partial p_C}\right)$
- The individual derivatives: $\frac{\partial l}{\partial p_i} = -\frac{y_i}{\mathbf{y}^T\mathbf{p}}$ for $i = 1, \dots, C$
- Putting it together:

$$\frac{\partial l}{\partial \mathbf{p}} = -\frac{\mathbf{y}^T}{\mathbf{y}^T\mathbf{p}}$$

Generic Backward Pass: Order of computations

Compute Gradient of node $\mathbf{p}$

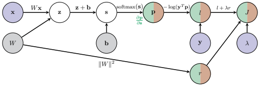


$$\boxed{l = -\log(\mathbf{y}^T\mathbf{p})}$$

$$\frac{\partial J}{\partial \mathbf{p}} = \frac{\partial J}{\partial l}\frac{\partial l}{\partial \mathbf{p}}$$

Generic Backward Pass: Order of computations

Compute Jacobian of node $\mathbf{p}$ w.r.t. its child $\mathbf{s}$



$$\boxed{\mathbf{p} = \exp(\mathbf{s}) / \left(\mathbf{1}^T\exp(\mathbf{s})\right)}$$

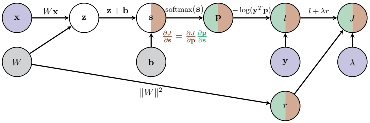
- The Jacobian we need to compute: $\frac{\partial \mathbf{p}}{\partial \mathbf{s}} = \begin{pmatrix} \frac{\partial p_1}{\partial s_1} & \cdots & \frac{\partial p_1}{\partial s_C} \\ \vdots & \vdots & \vdots \\ \frac{\partial p_C}{\partial s_1} & \cdots & \frac{\partial p_C}{\partial s_C} \end{pmatrix}$
- The individual derivatives:

$$\frac{\partial p_i}{\partial s_j} = \begin{cases} p_i(1-p_i) & \text{if } i = j \\ -p_i p_j & \text{otherwise} \end{cases}$$

- Putting it together in vector notation: $\frac{\partial \mathbf{p}}{\partial \mathbf{s}} = \text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T$

Generic Backward Pass: Order of computations

Compute Gradient of node $\mathbf{s}$

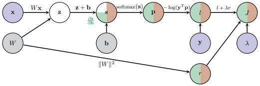


$$\boxed{\mathbf{p} = \exp(\mathbf{s}) / \left(\mathbf{1}^T \exp(\mathbf{s})\right)}$$

$$\frac{\partial J}{\partial \mathbf{s}} = \frac{\partial J}{\partial \mathbf{p}}\frac{\partial \mathbf{p}}{\partial \mathbf{s}}$$

Generic Backward Pass: Order of computations

Compute Jacobian of node $\mathbf{s}$ w.r.t. its child $\mathbf{b}$

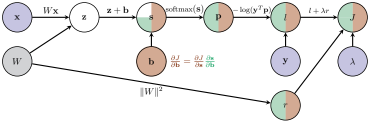


$$\boxed{\mathbf{s} = \mathbf{z} + \mathbf{b}}$$

- The Jacobian we need to compute: $\frac{\partial \mathbf{s}}{\partial \mathbf{b}} = \begin{pmatrix} \frac{\partial s_1}{\partial b_1} & \cdots & \frac{\partial s_1}{\partial b_C} \\ \vdots & \vdots & \vdots \\ \frac{\partial s_C}{\partial b_1} & \cdots & \frac{\partial s_C}{\partial b_C} \end{pmatrix}$
- The individual derivatives: $\frac{\partial s_i}{\partial b_j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: $\frac{\partial \mathbf{s}}{\partial \mathbf{b}} = I_C$ $\leftarrow$ the identity matrix of size $C \times C$

Generic Backward Pass: Order of computations

Compute Gradient of node $\mathbf{b}$

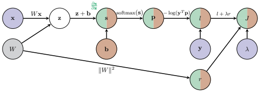


$$\boxed{\mathbf{s} = \mathbf{z} + \mathbf{b}}$$

gradient needed for mini-batch g.d.training as $\mathbf{b}$ parameter of the model $\rightarrow$ $$\frac{\partial J}{\partial \mathbf{b}} = \frac{\partial J}{\partial \mathbf{s}}\frac{\partial \mathbf{s}}{\partial \mathbf{b}}$$

Generic Backward Pass: Order of computations

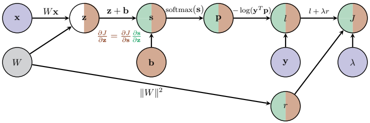
Compute Jacobian of node $\mathbf{s}$ w.r.t. its child $\mathbf{z}$



$$\boxed{\mathbf{s} = \mathbf{z} + \mathbf{b}}$$

- The Jacobian we need to compute: $\frac{\partial \mathbf{s}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial s_1}{\partial z_1} & \cdots & \frac{\partial s_1}{\partial z_C} \\ \vdots & \vdots & \vdots \\ \frac{\partial s_C}{\partial z_1} & \cdots & \frac{\partial s_C}{\partial z_C} \end{pmatrix}$
- The individual derivatives: $\frac{\partial s_i}{\partial z_j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: $\frac{\partial \mathbf{s}}{\partial \mathbf{z}} = I_C$ $\leftarrow$ the identity matrix of size $C \times C$

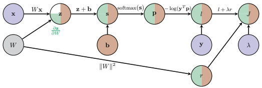
Compute Gradient of node z



$$\boxed{\mathbf{s} = \mathbf{z} + \mathbf{b}}$$

$$\frac{\partial J}{\partial \mathbf{z}} = \frac{\partial J}{\partial \mathbf{s}}\frac{\partial \mathbf{s}}{\partial \mathbf{z}}$$

Compute Jacobian of node z w.r.t. its child W



$$\boxed{\mathbf{z} = W\mathbf{x}}$$

- No consistent definition for "*Jacobian*" of vector w.r.t. matrix.
- Instead re-arrange W $(C \times d)$ into a vector vec(W) $(Cd \times 1)$

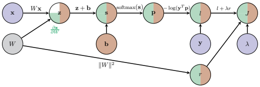
$$W = \begin{pmatrix} \mathbf{w}_1^T \\ \mathbf{w}_2^T \\ \vdots \\ \mathbf{w}_C^T \end{pmatrix} \quad \text{then} \quad \text{vec}(W) = \begin{pmatrix} \mathbf{w}_1 \\ \mathbf{w}_2 \\ \vdots \\ \mathbf{w}_C \end{pmatrix}$$

- Then

$$\mathbf{z} = \left(I_C \otimes \mathbf{x}^T\right) \text{vec}(W)$$

where $\otimes$ denotes the **Kronecker product** between two matrices.

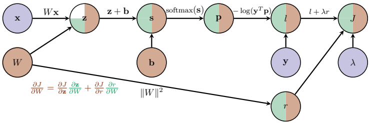
Compute Jacobian of node z w.r.t. its child W



$$\boxed{\mathbf{z} = W\mathbf{x} = \left(I_C \otimes \mathbf{x}^T\right) \text{vec}(W)}$$

- Let $\mathbf{v} = \text{vec}(W)$. Jacobian to compute: $\frac{\partial \mathbf{z}}{\partial \mathbf{v}} = \begin{pmatrix} \frac{\partial z_1}{\partial v_1} & \cdots & \frac{\partial z_1}{\partial v_{dC}} \\ \vdots & \vdots & \vdots \\ \frac{\partial z_C}{\partial v_1} & \cdots & \frac{\partial z_C}{\partial v_{dC}} \end{pmatrix}$
- The individual derivatives: $\frac{\partial z_i}{\partial v_j} = \begin{cases} x_{j-(i-1)d} & \text{if } (i-1)d+1 \le j \le id \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: $\frac{\partial \mathbf{z}}{\partial \mathbf{v}} = I_C \otimes \mathbf{x}^T$

Compute Gradient of node W



$$\boxed{\mathbf{z} = W\mathbf{x} = \left(I_C \otimes \mathbf{x}^T\right) \text{vec}(W)}$$

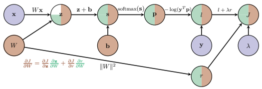
gradient needed for learning →

$$\frac{\partial J}{\partial \text{vec}(W)} = \frac{\partial J}{\partial \mathbf{z}}\frac{\partial \mathbf{z}}{\partial \text{vec}(W)} + \frac{\partial J}{\partial r}\frac{\partial r}{\partial \text{vec}(W)}$$
$$= \begin{pmatrix} g_1\mathbf{x}^T & g_2\mathbf{x}^T & \cdots & g_C\mathbf{x}^T \end{pmatrix} + 2\lambda\,\text{vec}(W)^T$$

if we set $\mathbf{g} = \frac{\partial J}{\partial \mathbf{z}}$.

Generic Backward Pass: Order of computations

Compute Gradient of node W



$$\boxed{\mathbf{z} = W\mathbf{x} = \left(I_C \otimes \mathbf{x}^T\right) \text{vec}(W)}$$

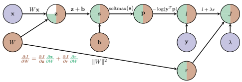
Can convert

$$\frac{\partial J}{\partial \text{vec}(W)} = \begin{pmatrix} g_1\mathbf{x}^T & g_2\mathbf{x}^T & \cdots & g_C\mathbf{x}^T \end{pmatrix} + 2\lambda\,\text{vec}(W)^T$$

(where $\mathbf{g} = \frac{\partial J}{\partial \mathbf{z}}$) from a vector $(1 \times Cd)$ back to a 2D matrix $(C \times d)$:

$$\frac{\partial J}{\partial W} = \begin{pmatrix} g_1\mathbf{x}^T \\ g_2\mathbf{x}^T \\ \vdots \\ g_C\mathbf{x}^T \end{pmatrix} + 2\lambda W = \mathbf{g}^T\mathbf{x}^T + 2\lambda W$$

Aggregating the Gradient computations



linear scoring function + SOFTMAX + cross-entropy loss + Regularization

$$\mathbf{g} = \frac{\partial J}{\partial l} = 1$$

$$\mathbf{g} \leftarrow \mathbf{g}\frac{\partial l}{\partial \mathbf{p}} = \left(-\frac{\mathbf{y}^T}{\mathbf{y}^T\mathbf{p}}\right) \quad \leftarrow \frac{\partial J}{\partial \mathbf{p}}$$

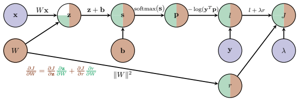
$$\mathbf{g} \leftarrow \mathbf{g}\frac{\partial \mathbf{p}}{\partial \mathbf{s}} = \mathbf{g}\left(\text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T\right) \quad \leftarrow \frac{\partial J}{\partial \mathbf{s}}$$

$$\mathbf{g} \leftarrow \mathbf{g}\frac{\partial \mathbf{s}}{\partial \mathbf{z}} = \mathbf{g}\,I_C \quad \leftarrow \frac{\partial J}{\partial \mathbf{z}}$$

Then

$$\frac{\partial J}{\partial \mathbf{b}} = \mathbf{g} \qquad\qquad \frac{\partial J}{\partial W} = \mathbf{g}^T\mathbf{x}^T + 2\lambda W$$

Aggregating the Gradient computations



linear scoring function + SOFTMAX + cross-entropy loss + Regularization

1. Let
$$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T\mathbf{p}}\left(\text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T\right)$$
2. The gradient of J w.r.t. the bias vector is the $1 \times C$ vector
$$\frac{\partial J}{\partial \mathbf{b}} = \mathbf{g}$$
3. The gradient of J w.r.t. the weight matrix W is the $C \times d$ matrix
$$\frac{\partial J}{\partial W} = \mathbf{g}^T\mathbf{x}^T + 2\lambda W$$

Gradient Computations for a mini-batch

- Have explicitly described the gradient computations for one training example $(\mathbf{x}, y)$.
- In general, want to compute the gradients of the cost function for a mini-batch $\mathcal{D}$.

$$\begin{aligned} J(\mathcal{D}, W, \mathbf{b}) &= L(\mathcal{D}, W, \mathbf{b}) + \lambda\|W\|^2 \\ &= \frac{1}{|\mathcal{D}|}\sum_{(\mathbf{x},y)\in\mathcal{D}} l(\mathbf{x}, y, W, \mathbf{b}) + \lambda\|W\|^2 \end{aligned}$$

- The gradients we need to compute are

$$\frac{\partial J(\mathcal{D}, W, \mathbf{b})}{\partial W} = \frac{\partial L(\mathcal{D}, W, \mathbf{b})}{\partial W} + 2\lambda W = \frac{1}{|\mathcal{D}|}\sum_{(\mathbf{x},y)\in\mathcal{D}} \frac{\partial l(\mathbf{x}, y, W, \mathbf{b})}{\partial W} + 2\lambda W$$

$$\frac{\partial J(\mathcal{D}, W, \mathbf{b})}{\partial \mathbf{b}} = \frac{\partial L(\mathcal{D}, W, \mathbf{b})}{\partial \mathbf{b}} = \frac{1}{|\mathcal{D}|}\sum_{(\mathbf{x},y)\in\mathcal{D}} \frac{\partial l(\mathbf{x}, y, W, \mathbf{b})}{\partial \mathbf{b}}$$

Gradient Computations for a mini-batch

linear scoring function + SOFTMAX + cross-entropy loss + Regularization

- Compute gradients of l w.r.t. $W, \mathbf{b}$ for each $(\mathbf{x}, y) \in \mathcal{D}^{(t)}$:
  - Set all entries in $\frac{\partial L}{\partial \mathbf{b}}$ and $\frac{\partial L}{\partial W}$ to zero.
  - for $(\mathbf{x}, y) \in \mathcal{D}^{(t)}$
    1. Let
    $$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T\mathbf{p}}\left(\text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T\right)$$
    2. Add gradient of l w.r.t. $\mathbf{b}$ computed at $(\mathbf{x}, y)$
    $$\frac{\partial L}{\partial \mathbf{b}} \mathrel{+}= \mathbf{g}$$
    3. Add gradient of l w.r.t. W computed at $(\mathbf{x}, y)$
    $$\frac{\partial L}{\partial W} \mathrel{+}= \mathbf{g}^T\mathbf{x}^T$$
  - Divide by the number of entries in $\mathcal{D}^{(t)}$:
  $$\frac{\partial L}{\partial W} \mathrel{/}= |\mathcal{D}^{(t)}|, \qquad \frac{\partial L}{\partial \mathbf{b}} \mathrel{/}= |\mathcal{D}^{(t)}|$$
- Add the gradient for the regularization term
$$\frac{\partial J}{\partial W} = \frac{\partial L}{\partial W} + 2\lambda W, \qquad \frac{\partial J}{\partial \mathbf{b}} = \frac{\partial L}{\partial \mathbf{b}}$$