Topics:

- Neural Networks
- Backpropagation


## CS 4644-DL / 7643-A ZSOLT KIRA

- Assignment 1 out!
- Due Feb 5 ${ }^{\text {th }}$
- Start now, start now, start now!
- Start now, start now, start now!
- Start now, start now, start now!
- Piazza
- Be active!!!
- Extra credit!
- Office hours
- Assignment (@41) and matrix calculus (@46)

Example with an image with 4 pixels, and 3 classes (cat/dog/ship)


Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

- We can find the steepest descent direction by computing the derivative (gradient):

$$
f^{\prime}(a)=\lim _{h \rightarrow 0} \frac{f(a+\boldsymbol{h})-\boldsymbol{f}(\boldsymbol{a})}{\boldsymbol{h}}
$$

- Steepest descent direction is the negative gradient
- Intuitively: Measures how the function changes as the argument a changes by a small step size
- As step size goes to zero
- In Machine Learning: Want to know how the loss function changes as weights are varied
- Can consider each parameter separately by taking partial derivative of loss function with respect to that parameter



## Derivatives

## This idea can be turned into an algorithm (gradient descent)

- Choose a model: $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{W})=\mathrm{Wx}$
- Choose loss function: $L_{i}=\left|\boldsymbol{y}-\boldsymbol{W} \boldsymbol{x}_{\boldsymbol{i}}\right|^{2}$
- Calculate partial derivative for each parameter: $\frac{\partial L}{\partial w_{i}}$
- Update the parameters: $\boldsymbol{w}_{\boldsymbol{i}}=\boldsymbol{w}_{\boldsymbol{i}}-\frac{\partial L}{\partial w_{i}}$
- Add learning rate to prevent too big of a step: $\boldsymbol{w}_{\boldsymbol{i}}=\boldsymbol{w}_{\boldsymbol{i}}-\alpha \frac{\partial L}{\partial \boldsymbol{w}_{i}}$
- Repeat (from Step 3)

Often, we only compute the gradients across a small subset of data

- Full Batch Gradient Descent

$$
L=\frac{1}{N} \sum L\left(f\left(x_{i}, W\right), y_{i}\right)
$$

$$
L=\frac{1}{M} \sum L\left(f\left(x_{i}, W\right), y_{i}\right)
$$

- Where M is a subset of data
- We iterate over mini-batches:
- Get mini-batch, compute loss, compute derivatives, and take a set
http://demonstrations.wolfram.com/VisualizingTheGradientVector/

original W


## negative gradient direction

## For some functions, we can analytically derive the partial derivative <br> Example: <br> Derivation of Update Rule

## Function

$f\left(w, x_{i}\right)=w^{T} x_{i} \quad\left(y_{i}-w^{T} x_{i}\right)^{2}$
(Assume $\boldsymbol{w}$ and $\mathbf{x}_{\mathbf{i}}$ are column vectors, so same as $\boldsymbol{w} \cdot \boldsymbol{x}_{\boldsymbol{i}}$ )
Dataset: N examples (indexed by $k$ )
Update Rule
$w_{j} \leftarrow w_{j}+2 \eta \sum_{k=1}^{N} \delta_{k} x_{k j}$

Loss
$\mathrm{L}=\sum_{k=1}^{N}\left(y_{k}-w^{T} x_{k}\right)^{2}$

Gradient descent tells us we should update $\boldsymbol{w}$ as follows to minimize $L$ :
$w_{j} \leftarrow w_{j}-\eta \frac{\partial L}{\partial w_{j}}$

So what's $\frac{\partial L}{\partial w_{j}}$ ?

$$
\begin{aligned}
& \frac{\partial L}{\partial w_{j}}=\sum_{k=1}^{N} \frac{\partial}{\partial w_{j}}\left(y_{k}-w^{T} x_{k}\right)^{2} \\
& =\sum_{k=1}^{N} 2\left(y_{k}-w^{T} x_{k}\right) \frac{\partial}{\partial w_{j}}\left(y_{k}-w^{T} x_{k}\right) \\
& =-2 \sum_{k=1}^{N} \delta_{k} \frac{\partial}{\partial w_{j}} \boldsymbol{w}^{T} \boldsymbol{x}_{\boldsymbol{k}} \\
& =-2 \sum_{k=1}^{N} \delta_{k} \frac{\partial}{\partial w_{j}} \sum_{i=1}^{m} w_{i} x_{k i} \\
& =-2 \sum_{k=1}^{N} \delta_{k} x_{k j}
\end{aligned}
$$

If we add a non-linearity (sigmoid), derivation is more complex

$$
\sigma(x)=\frac{1}{1+e^{-x}}
$$

First, one can derive that: $\boldsymbol{\sigma}^{\prime}(\boldsymbol{x})=\boldsymbol{\sigma}(\boldsymbol{x})(\mathbf{1}-\boldsymbol{\sigma}(\boldsymbol{x}))$

$$
\begin{aligned}
\mathrm{f}(\mathrm{x}) & =\sigma\left(\sum_{k} w_{k} x_{k}\right) \\
\mathrm{L} & =\sum_{i}\left(y_{i}-\sigma\left(\sum_{k} w_{k} x_{i k}\right)\right)^{2} \\
\frac{\partial L}{\partial w_{j}} & =\sum_{i} 2\left(y_{i}-\sigma\left(\sum_{k} w_{k} x_{i k}\right)\right)\left(-\frac{\partial}{\partial w_{j}} \sigma\left(\sum_{k} w_{k} x_{i k}\right)\right) \\
& =\sum_{i}-2\left(y_{i}-\sigma\left(\sum_{k} w_{k} x_{i k}\right)\right) \sigma^{\prime}\left(\sum_{k} w_{k} x_{i k}\right) \frac{\partial}{\partial w_{j}} \sum_{k} w_{k} x_{i k} \\
& =\sum_{i}-2 \delta_{i} \sigma\left(\mathbf{d}_{i}\right)\left(1-\sigma\left(\mathbf{d}_{i}\right)\right) x_{i j}
\end{aligned}
$$

where $\quad \delta_{i}=y_{i}-\mathrm{f}\left(x_{i}\right) \quad d_{i}=\sum w_{k} x_{i k}$


The sigmoid perception update rule:

$$
\begin{gathered}
w_{j} \leftarrow w_{j}+2 \eta \sum_{k=1}^{N} \delta_{i} \sigma_{i}\left(1-\sigma_{i}\right) x_{i j} \\
\text { where } \sigma_{i}=\sigma\left(\sum_{j=1}^{m} w_{j} x_{i j}\right) \\
\delta_{i}=y_{i}-\sigma_{i}
\end{gathered}
$$

A linear classifier can be broken down into:

- Input
- A function of the input
- A loss function

It's all just one function that can be decomposed into building blocks


The same two-layered neural network corresponds to adding another weight matrix

- We will prefer the linear algebra view, but use some terminology from neural networks (\& biology)

hidden layer

$$
\begin{array}{cl}
x & W_{1} \\
& = \\
f\left(x, W_{1}, W_{2}\right) & =\sigma\left(W_{2} \sigma\left(W_{1} x\right)\right)
\end{array}
$$

Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Large (deep) networks can be built by adding more and more layers
Three-layered neural networks can represent any function

- The number of nodes could grow unreasonably (exponential or worse) with respect to the complexity of the function
We will show them without edges:



$$
f\left(x, W_{1}, W_{2}, W_{3}\right)=\sigma\left(W_{2} \sigma\left(W_{1} x\right)\right)
$$

Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

## Adding More Layers!

## Demo

- http://playground.tensorflow.org



## Computation Graphs

Functions can be made arbitrarily complex (subject to memory and computational limits), e.g.:

$$
f(x, W)=\sigma\left(W _ { 5 } \sigma \left(W _ { 4 } \sigma \left(W_{3} \sigma\left(W_{2} \sigma\left(W_{1} x\right)\right)\right.\right.\right.
$$

We can use any type of differentiable function (layer) we want!

- At the end, add the loss function

Composition can have some structure


The world is compositional!

We want our model to reflect this
Empirical and theoretical evidence that it makes learning complex functions easier

Note that prior state of art engineered features often had this compositionality as well

```
VISION
    pixels }=>\mathrm{ edge }=>\mathrm{ texton }=>\mathrm{ motif }=>\mathrm{ part }=>\mathrm{ object
SPEECH
    sample }=>\begin{array}{c}{\mathrm{ spectral }}\end{array}=>\mathrm{ formant }=>\mathrm{ motif }=>\mathrm{ phone }=>\mathrm{ word
NLP
    character }=>\mathrm{ word }=>\mathrm{ NP/VP/.. }=>\mathrm{ clause }=>\mathrm{ sentence }=>\mathrm{ story
```

- Pixels -> edges -> object parts -> objects


## Compositionality

- We are learning complex models with significant amount of parameters (millions or billions)
- How do we compute the gradients of the loss (at the end) with respect to internal parameters?
- Intuitively, want to understand how small changes in weight deep inside are propagated to affect the loss function at the end


Given a library of simple functions


Adapted from slides by: Marc'Aurelio Ranzato, Yann LeCun

To develop a general algorithm for this, we will view the function as a computation graph

Graph can be any directed acyclic graph (DAG)

- Modules must be differentiable to support gradient computations for gradient descent

A training algorithm will then process this graph, one module at a time


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

## Directed Acyclic Graphs (DAGs)

- Exactly what the name suggests
- Directed edges
- No (directed) cycles
- Underlying undirected cycles okay



## Directed Acyclic Graphs (DAGs)

- Concept
- Topological Ordering


Directed Acyclic Graphs (DAGs)


$$
f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$



$$
-\log \left(\frac{1}{1+e^{-w \cdot x}}\right)
$$



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun
Machine Learning Example

## Backpropagation

## Step 1: Compute Loss on Mini-Batch: Forward Pass



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

## Neural Network Training

## Step 1: Compute Loss on Mini-Batch: Forward Pass



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

## Neural Network Training

## Step 1: Compute Loss on Mini-Batch: Forward Pass



Note that we must store the intermediate outputs of all layers!

- This is because we will need them to compute the gradients (the gradient equations will have terms with the output values in them)


## Step 1: Compute Loss on Mini-Batch: Forward Pass <br> Step 2: Compute Gradients wrt parameters: Backward Pass



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

## Step 1: Compute Loss on Mini-Batch: Forward Pass <br> Step 2: Compute Gradients wrt parameters: Backward Pass



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## Step 1: Compute Loss on Mini-Batch: Forward Pass <br> Step 2: Compute Gradients wrt parameters: Backward Pass



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## Neural Network Training

We want to compute: $\left\{\frac{\partial L}{\partial \boldsymbol{h}^{\ell-1}}, \frac{\partial L}{\partial W}\right\}$


- We will use the chain rule to do this:

Chain Rule: $\frac{\partial z}{\partial x}=\frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

## Step 1: Compute Loss on Mini-Batch: Forward Pass

Step 2: Compute Gradients wrt parameters: Backward Pass
Step 3: Use gradient to update all parameters at the end


$$
w_{i}=w_{i}-\alpha \frac{\partial L}{\partial w_{i}} \quad \begin{aligned}
& \text { Backpropagation is the application of } \\
& \begin{array}{l}
\text { gradient descent to a computation } \\
\text { graph via the chain rule! }
\end{array}
\end{aligned}
$$

Given this computation graph, the training algorithm will:

- Calculate the current model's outputs (called the forward pass)
- Calculate the gradients for each module (called the backward pass)
Backward pass is a recursive algorithm that:
- Starts at loss function where we know how to calculate the gradients
- Progresses back through the modules
- Ends in the input layer where we do not need gradients (no parameters)
This algorithm is called backpropagation



## Overview of Training

In the backward pass, we seek to calculate the gradients of the loss with respect to the module's parameters

- Assume that we have the gradient of the loss with respect to the module's outputs (given to us by upstream module)
- We will also pass the gradient of the loss with respect to the module's inputs
- This is not required for update the module's weights, but passes the gradients back to the previous module



## Problem:

- We can compute local gradients: $\left\{\frac{\partial h^{\ell}}{\partial \boldsymbol{h}^{\ell-1}}, \frac{\partial \boldsymbol{h}^{\ell}}{\partial W}\right\}$
- We are given: $\frac{\partial L}{\partial h^{\ell}}$
- Compute: $\left\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\right\}$
- We can compute local gradients: $\left\{\frac{\partial h^{\ell}}{\partial \boldsymbol{h}^{\ell-1}}, \frac{\partial \boldsymbol{h}^{\ell}}{\partial W}\right\}$

This is just the derivative of our function with respect to its parameters and inputs!

Example: If $\boldsymbol{h}^{\ell}=\boldsymbol{W} \boldsymbol{h}^{\ell-1}$

$$
\begin{aligned}
& \text { then } \frac{\partial \boldsymbol{h}^{\ell}}{\partial \boldsymbol{h}^{\ell-1}}=\boldsymbol{W} \\
& \text { (a sparse matrix with } \\
& \text { and } \frac{\partial \boldsymbol{h}^{\ell}}{\partial w_{i}}=\boldsymbol{h}^{\ell-1, T} \\
& \text { in the } i \text {-th row }
\end{aligned}
$$

We want to to compute: $\left\{\frac{\partial L}{\partial \boldsymbol{h}^{\ell-1}}, \frac{\partial L}{\partial W}\right\}$


- We will use the chain rule to do this:

Chain Rule: $\frac{\partial z}{\partial x}=\frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

- We will use the chain rule to compute: $\left\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\right\}$
- Gradient of loss w.r.t. inputs: $\frac{\partial L}{\partial h^{\ell-1}}=\frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$

Given by upstream module (upstream gradient)

- Gradient of loss w.r.t. weights: $\frac{\partial L}{\partial W}=\frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial W}$


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

## Backpropagation: a simple example

$$
f(x, y, z)=(x+y) z
$$

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## Backpropagation: a simple example

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\begin{aligned}
& f(x, y, z)=(x+y) z \\
& \text { e.g. } x=-2, y=5, z=-4
\end{aligned}
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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\end{aligned}
$$



## Backpropagation: a simple example



## Backpropagation: a simple example



## Patterns in backward flow



## Patterns in backward flow

Q: What is an add gate?


## Patterns in backward flow

add gate: gradient distributor


## Patterns in backward flow

add gate: gradient distributor Q: What is a max gate?


## Patterns in backward flow

add gate: gradient distributor max gate: gradient router


## Patterns in backward flow

add gate: gradient distributor max gate: gradient router Q: What is a mul gate?


## Patterns in backward flow

add gate: gradient distributor max gate: gradient router mul gate: gradient switcher


## Gradients add at branches



Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231 n

## Duality in Fprop and Bprop



## Deep Learning $=$ Differentiable Programming

- Computation = Graph
- Input = Data + Parameters
- Output = Loss
- Scheduling = Topological ordering
- What do we need to do?
- Generic code for representing the graph of modules
- Specify modules (both forward and backward function)


## Modularized implementation: forward / backward API

## Graph (or Net) object (rough psuedo code)



```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
        gate.backward() # little piece of backprop (chain rule applied)
    return inputs_gradients
```


## Modularized implementation: forward / backward API



[^0]
## Modularized implementation: forward / backward API



```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
```

```
        dx = self.y * dz # [dz/dx * dL/dz]
```

        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
    ```
        return [dx, dy]
```

(x,y,z are scalars)

## Example: Caffe layers

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## Caffe Sigmoid Layer



Batches of data are matrices or tensors (multi-dimensional matrices) Examples:

- Each instance is a vector of size $m$, our batch is of size [ $\boldsymbol{B} \times \boldsymbol{m}$ ]
- Each instance is a matrix (e.g. grayscale image) of size $\boldsymbol{W} \times \boldsymbol{H}$, our batch is [ $\boldsymbol{B} \times \boldsymbol{W} \times \boldsymbol{H}$ ]
- Each instance is a multi-channel matrix (e.g. color image with $\mathrm{R}, \mathrm{B}, \mathrm{G}$ channels) of size $\boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}$, our batch is $[\boldsymbol{B} \times \boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}]$
Jacobians become tensors which is complicated
- Instead, flatten input to a vector and get a vector of derivatives!
- In practice, figure out Jacobians for simpler items (scalars, vectors), figure out pattern, and slice or index appropriate elements to create Jacobians

$$
\left[\begin{array}{cccc}
x_{11} & x_{12} & \cdots & x_{1 n} \\
x_{21} & x_{22} & \cdots & x_{2 n} \\
\vdots & \vdots & \ddots & \vdots \\
x_{n 1} & x_{n 2} & \cdots & x_{n n}
\end{array}\right]
$$

Flatten
[
$\left[\begin{array}{c}x_{11} \\ x_{12} \\ \vdots \\ x_{21} \\ x_{22} \\ \vdots \\ x_{n 1} \\ \vdots \\ x_{n n}\end{array}\right]$




[^0]:    Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231 n

