Topics:

- Gradient Descent
- Neural Networks

CS 4644-DL / 7643-A ZSOLT KIRA

- Assignment 1 out!
- Due Feb $2^{\text {nd }}$ (with grace period Feb $4^{\text {th }}$ )
- Start now, start now, start now!
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- Start now, start now, start now!
- Piazza
- Be active!!!
- Office hours
- Lots of special topics (e.g. Assignment 1, Matrix Calculus, etc. )
- Note: Course will start to get math heavy!
- Input (and representation)
- Functional form of the model
- Including parameters
- Performance measure to improve
- Loss or objective function
Algorithm for finding best parameters
- Optimization algorithm


Data: Image


Features: Histogram


Input: Vector

- Functional form of the model: Softmax(Wx)

Performance measure to improve: Cross-Entropy
Algorithm for finding best parameters: Gradient Descent
Compute $\frac{\partial L}{\partial w_{i}}$

- Update Weights $\boldsymbol{w}_{\boldsymbol{i}}=\boldsymbol{w}_{\boldsymbol{i}}-\alpha \frac{\partial L}{\partial w_{i}}$

We know how to compute the model output and loss function

## Several ways to compute $\frac{\partial L}{\partial w_{i}}$

Manual differentiation- Symbolic differentiation

Numerical differentiation

- Automatic differentiation



## Computing Gradients

## For some functions, we can analytically derive the partial derivative

## Example:

Function
$f\left(w, x_{i}\right)=w^{T} x_{i}$

Loss

$$
\sum_{i=1}^{N}\left(y_{i}-w^{T} x_{i}\right)^{2}
$$

(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 $i$ )
Update Rule
$w_{j} \leftarrow w_{j}+2 \alpha \sum_{i=1}^{N} \delta_{i} x_{i j}$

## Derivation of Update Rule

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

$$
\frac{\partial L}{\partial w_{j}}=\sum_{i=1}^{N} \frac{\partial}{\partial w_{j}}\left(y_{i}-w^{T} x_{i}\right)^{2}
$$

$$
=\sum_{i=1}^{N} 2\left(y_{i}-w^{T} x_{i}\right) \frac{\partial}{\partial w_{j}}\left(y_{i}-w^{T} x_{i}\right)
$$

$$
=-2 \sum_{i=1}^{N} \delta_{i} \frac{\partial}{\partial w_{j}} w^{T} x_{i}
$$

$$
=-2 \sum_{i=1}^{N} \delta_{i} \frac{\partial}{\partial w_{j}} \sum_{k=1} w_{k} x_{i k}
$$

$$
=-2 \sum_{i=1}^{N} \delta_{i} x_{i j}
$$

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

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

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

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

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:

$$
\begin{array}{r}
w_{j} \leftarrow w_{j}+2 \alpha \sum_{k=1}^{N} \delta_{i} \sigma_{i}\left(1-\sigma_{i}\right) x_{i j} \\
\text { where } \quad \sigma_{i}=\sigma\left(\sum_{j=1}^{d} w_{j} x_{i j}\right) \\
\delta_{i}=y_{i}-\sigma_{i}
\end{array}
$$

## Neural Network View of a Linear Classifier

A simple neural network has similar structure as our linear classifier:

- A neuron takes input (firings) from other neurons (-> input to linear classifier)
- The inputs are summed in a weighted manner (-> weighted sum)
- Learning is through a modification of the weights
- If it receives enough input, it "fires" (threshold or if weighted sum plus bias is high enough)


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

As we did before, the output of a


## Sigmoid <br> Activation <br> Function <br> $\frac{1}{1+e^{-x}}$

Impulses carried toward cell body


axon from a neuron


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

We can have multiple neurons connected to the same input

Corresponds to a multi-class classifier Each output node outputs the score for a class

$$
f(x, W)=\sigma(W x+b)\left[\begin{array}{lllll}
w_{11} & w_{12} & \cdots & w_{1 m} & b 1 \\
w_{21} & w_{22} & \cdots & w_{2 m} & b 2 \\
w_{21} & w_{22} & \cdots & w_{3 m} & b 3
\end{array}\right]
$$

Often called fully connected layers

output layer

- Also called a linear projection layer
- Each input/output is a neuron (node)
- A linear classifier (+ optional nonlinearity) is called a fully connected layer
- Connections are represented as edges
- Output of a particular neuron is referred to as activation
- 

This will be expanded as we view
 computation in a neural network as a graph

We can stack multiple layers together

- Input to second layer is output of first layer
Called a 2-layered neural network (input is not counted)
Because the middle layer is neither input or output, and we don't know what their values represent, we call them hidden layers
- We will see that they end up learning effective features

This increases the representational power
 of the function!

- Two layered networks can represent any continuous function

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)


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


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:


## Adding More Layers!

## 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


Adding Even More Layers

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

```
SPEECH
    sample }=>\underset{\mathrm{ spectral }}{\mathrm{ band }}=>\mathrm{ formant }=>\mathrm{ motif }=>\mathrm{ phone }=>\mathrm{ word
    sample }=>\underset{\mathrm{ spectral }}{\mathrm{ band }}=>\mathrm{ formant }=>\mathrm{ motif }=>\mathrm{ phone }=>\mathrm{ word
NLP
NLP
    character }=>\mathrm{ word }=>\mathrm{ NP/VP/.. }>\mathrm{ clause }=>\mathrm{ sentence }=>\mathrm{ story
```

```
    character }=>\mathrm{ word }=>\mathrm{ NP/VP/.. }>\mathrm{ clause }=>\mathrm{ sentence }=>\mathrm{ story
```

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

\section*{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

\section*{A General Framework}

\section*{Directed Acyclic Graphs (DAGs)}
- Exactly what the name suggests
- Directed edges
- No (directed) cycles
- Underlying undirected cycles okay


\section*{Directed Acyclic Graphs (DAGs)}
- Concept
- Topological Ordering


\section*{Directed Acyclic Graphs (DAGs)}


\section*{Backpropagation}

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


\section*{Step 1: Compute Loss on Mini-Batch: Forward Pass}


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\section*{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)

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


\section*{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: \(\left\{\frac{\partial L}{\partial h^{\ell-1}} \frac{\partial L}{\partial W}\right\}\)

\section*{Backward Pass Computations}

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: \(\frac{\partial z}{\partial x}=\frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}\)
- We can compute local gradients: \(\left\{\frac{\partial h^{\ell}}{\partial h^{\ell-1}}, \frac{\partial h^{\ell}}{\partial W}\right\}\)

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

Example: If \(\boldsymbol{h}^{\ell}=W \boldsymbol{h}^{\ell-1}\)
\[
\begin{aligned}
& \text { then } \frac{\partial h^{\ell}}{\partial h^{\ell-1}}=W \\
& \text { and } \frac{\partial \boldsymbol{h}_{i}^{\ell}}{\partial w_{i}}=\boldsymbol{h}^{\ell-1, T}
\end{aligned}
\]
- 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: \(\frac{\partial L}{\partial W}=\frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial W}\)


\section*{Step 1: Compute Loss on Mini-Batch: Forward Pass \\ Step 2: Compute Gradients wrt parameters: Backward Pass}


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\section*{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

\[
w_{i}=w_{i}-\alpha \frac{\partial L}{\partial w_{i}}
\]

Backpropagation is the application of gradient descent to a computation graph via the chain rule!

\section*{Backpropagation: a simple example}
\[
f(x, y, z)=(x+y) z
\]

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

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\section*{Backpropagation: a simple example}


\section*{Backpropagation: a simple example}


\section*{Patterns in backward flow}


\section*{Patterns in backward flow}

Q: What is an add gate?


\section*{Patterns in backward flow}
add gate: gradient distributor


\section*{Patterns in backward flow}
add gate: gradient distributor
Q: What is a max gate?


\section*{Patterns in backward flow}
add gate: gradient distributor max gate: gradient router


\section*{Patterns in backward flow}
add gate: gradient distributor max gate: gradient router Q: What is a mul gate?


\section*{Patterns in backward flow}
add gate: gradient distributor max gate: gradient router mul gate: gradient switcher


\section*{Gradients add at branches}


\section*{Duality in Fprop and Bprop}


\section*{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)

\section*{Modularized implementation: forward / backward API}

\section*{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


\title{
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]
dy = self.x * dz \# [dz/dy * dL/dz]
return [dx, dy]

```

\section*{Example: Caffe layers}
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\section*{Caffe Sigmoid Layer}
```

