Topics:

- Neural Networks
- Backpropagation

CS 4644-DL / 7643-A ZSOLT KIRA

• Assignment 1 out!

- Due Feb 5th
- 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
 - <u>Assignment</u> (@41) and <u>matrix calculus</u> (@46)

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



Stretch pixels into column

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



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

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

- 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

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

• Choose a model:
$$f(x, W) = Wx$$

Choose loss function: $L_i = |y - Wx_i|^2$

Calculate partial derivative for each parameter: $\frac{\partial L}{\partial w_i}$

• Update the parameters:
$$w_i = w_i - \frac{\partial L}{\partial w_i}$$

• Add learning rate to prevent too big of a step: $w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$

Repeat (from Step 3)

Gradient Descent

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

Full Batch Gradient Descent

$$L = \frac{1}{N} \sum L\left(f(x_i, W), y_i\right)$$

Mini-Batch Gradient Descent

$$L = \frac{1}{M} \sum L(f(x_i, W), y_i)$$

- 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/

For some functions, we can analytically derive the partial derivative

 $w_j \leftarrow w_j - \eta \frac{\partial L}{\partial w_i}$

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

Example:

Loss Function $f(w, x_i) = w^T x_i \qquad (y_i - w^T x_i)^2$

(Assume w and \mathbf{x}_i are column vectors, so same as $w \cdot x_i$)

Dataset: N examples (indexed by k)

Update Rule $w_j \leftarrow w_j + 2\eta \sum_{k=4}^{N} \delta_k x_{kj}$

$$L = \sum_{k=1}^{N} (y_k - w^T x_k)^2 \qquad \frac{\partial L}{\partial w_j} = \sum_{k=1}^{N} \frac{\partial}{\partial w_j} (y_k - w^T x_k)^2$$
Gradient descent tells us
we should update **w** as
follows to minimize *L*:

$$w_j \leftarrow w_j - \eta \frac{\partial L}{\partial w_j}$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} w^T x_k$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{M} w_i x_{ki}$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{M} w_i x_{ki}$$

$$= -2 \sum_{k=1}^{N} \delta_k x_{kj}$$

Derivation of Update Rule

Manual Differentiation



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

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

First, one can derive that: $\sigma'(x) = \sigma(x)(1 - \sigma(x))$

$$f(\mathbf{x}) = \sigma\left(\sum_{k} w_{k} x_{k}\right)$$

$$L = \sum_{i} \left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right)^{2}$$

$$\frac{\partial L}{\partial w_{j}} = \sum_{i} 2\left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right) \left(-\frac{\partial}{\partial w_{j}} \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right)$$

$$= \sum_{i} -2\left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right) \sigma'\left(\sum_{k} w_{k} x_{ik}\right) \frac{\partial}{\partial w_{j}} \sum_{k} w_{k} x_{ik}$$

$$= \sum_{i} -2\delta_{i}\sigma(\mathbf{d}_{i})(1 - \sigma(\mathbf{d}_{i}))x_{ij}$$
where $\delta_{i} = y_{i} - \mathbf{f}(x_{i})$ $d_{i} = \sum w_{k} x_{ik}$



The sigmoid perception update rule:



Adding a Non-Linear Function

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A linear classifier can be broken down into:

- lnput
- 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)



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**:





$f(x, W_1, W_2, W_3) = \sigma(W_2 \sigma(W_1 x))$

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



Adding More Layers!

Demo

<u>http://playground.tensorflow.org</u>





Computation Graphs



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

$$f(x,W) = \sigma(W_5\sigma(W_4\sigma(W_3\sigma(W_2\sigma(W_1x)))$$

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



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Pixels -> edges -> object parts -> objects



- 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



Computing Gradients in Complex Function





Given a library of simple functions





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







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Directed Acyclic Graphs (DAGs)

- Concept
 - Topological Ordering









Directed Acyclic Graphs (DAGs)



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Backpropagation



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







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







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 PassStep 2: Compute Gradients wrt parameters: Backward Pass







Step 1: Compute Loss on Mini-Batch: Forward PassStep 2: Compute Gradients wrt parameters: Backward Pass







Step 1: Compute Loss on Mini-Batch: Forward PassStep 2: Compute Gradients wrt parameters: Backward Pass







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



We will use the *chain rule* to do this:

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

Computing the Gradients of Loss



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!





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**



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun



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: $\{\frac{\partial h^{\ell}}{\partial h^{\ell-1}}, \frac{\partial h^{\ell}}{\partial W}\}$

• We are given:
$$\frac{\partial L}{\partial h^{\ell}}$$

• Compute: $\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\}$





- We can compute **local gradients**: $\{\frac{\partial h^{\ell}}{\partial h^{\ell-1}}, \frac{\partial h^{\ell}}{\partial W}\}$
- This is just the derivative of our function with respect to its parameters and inputs!

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

then
$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = W$$

(a sparse matrix with
and $\frac{\partial h^{\ell}}{\partial w_i} = \frac{h^{\ell-1,T}}{h^{\ell-1,T}}$
in the *i*-th row

Computing the Local Gradients: Example






We will use the *chain rule* to do this:

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

Computing the Gradients of Loss





• Gradient of loss w.r.t. inputs: $\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$

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



Given by upstream module (upstream gradient)

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Computing the Gradients of Loss



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



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

Justin Johnson, Serena Yeung, CS 231n

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





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

e.g. x = -2, y = 5, z = -4





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

e.g. x = -2, y = 5, z = -4



Want:
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$

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Want:
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$

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Q: What is an **add** gate?





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add gate: gradient distributor





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add gate: gradient distributor

Q: What is a **max** gate?





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add gate: gradient distributormax gate: gradient router





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add gate: gradient distributormax gate: gradient routerQ: What is a mul gate?





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add gate: gradient distributormax gate: gradient routermul gate: gradient switcher





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Gradients add at branches





Duality in Fprop and Bprop





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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

C



Graph (or Net) object (rough psuedo code)

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



Modularized implementation: forward / backward API





Modularized implementation: forward / backward API



lass Mu	<pre>iltiplyGate(object):</pre>
def	forward(x,y):
	$z = x^*y$
	<pre>self.x = x # must keep these around!</pre>
	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]



Example: Caffe layers

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a year ago 11 months ago 11 months ago 11 months ago 11 months ago a year ago a year ago 11 months ago 11 months ago 3 months ago a year ago





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

- Each instance is a vector of size m, our batch is of size $[B \times m]$
- Each instance is a matrix (e.g. grayscale image) of size $W \times H$, our batch is $[B \times W \times H]$
- Each instance is a multi-channel matrix (e.g. color image with R,B,G channels) of size $C \times W \times H$, our batch is $[B \times C \times W \times H]$

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








Fully Connected (FC) Layer: Forward Function





Fully Connected (FC) Layer

