

10-301/601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

Backpropagation + RNNs

Matt Gormley Lecture 13 Feb. 28, 2022

Reminders

- **Homework 5: Neural Networks**
	- **Out: Sun, Feb 27**
	- **Due: Fri, Mar 18 at 11:59pm**

A 1-Hidden Layer Neural Network

TRAINING A NEURAL NETWORK

Backpropagation

7

SGD with Backprop

Example: 1-Hidden Layer Neural Network

A 1-Hidden Layer Neural Network

FORWARD COMPUTATION FOR A NEURAL NETWORK

SGD with Backprop

Example: 1-Hidden Layer Neural Network

Backpropagation

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A 1-Hidden Layer Neural Network

BACKPROPAGATION FOR A NEURAL NETWORK

Backpropagation

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Backpropagation

Case 2: Neural Network

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

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

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

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

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

Backward
\n
$$
\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1-y^*)}{y-1}
$$
\n
$$
\frac{dJ}{db} = \frac{dJ}{dy} \frac{dy}{db}, \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}
$$
\n
$$
\frac{dJ}{d\beta_j} = \frac{dJ}{db} \frac{db}{d\beta_j}, \frac{db}{d\beta_j} = z_j
$$
\n
$$
\frac{dJ}{dz_j} = \frac{dJ}{db} \frac{db}{dz_j}, \frac{db}{dz_j} = \beta_j
$$
\n
$$
\frac{dJ}{da_j} = \frac{dJ}{dz_j} \frac{dz_j}{da_j}, \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}
$$
\n
$$
\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j} \frac{da_j}{d\alpha_{ji}}, \frac{da_j}{d\alpha_{ji}} = x_i
$$
\n
$$
\frac{dJ}{dx_i} = \sum_{j=0}^{D} \frac{dJ}{da_j} \frac{da_j}{dx_i}, \frac{da_j}{dx_i} = \alpha_{ji}
$$

Backpropagation

Derivative of a Sigmoid

First suppose that

 \equiv

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

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

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

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

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

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

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

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

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

 $= s(1-s)$ (9)

Backpropagation

Backpropagation

SGD with Backprop

Example: 1-Hidden Layer Neural Network

THE BACKPROPAGATION ALGORITHM

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

- 1. Write an **algorithm** for evaluating the function y = f(**x**). The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph"**)
- 2. Visit each node in **topological order.**
For variable u_i with inputs v₁,..., v_N
	- a. Compute $u_i = g_i(v_1, ..., v_N)$
	- b. Store the result at the node

Backward Computation (Version A)

-
- **1. Initialize** $dy/dy = 1$.
2. Visit each node v_i in **reverse topological order**.

2. Visit each node v_j in **reverse topological order**.
Let u₁,..., u_M denote all the nodes with v_i as an input Assuming that $y = h(\mathbf{u}) = h(u_1, \dots, u_M)$ and $\mathbf{u} = \mathbf{g}(\mathbf{v})$ or equivalently $\mathbf{u}_i = \mathbf{g}_i(\mathbf{v}_1,\dots,\mathbf{v}_j,\dots,\mathbf{v}_N)$ for all i

- a. We already know dy/du_i for all i
- b. Compute $\frac{dy}{dv_i}$ as below (Choice of algorithm ensures computing (du_i/dv_j) is easy)

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

Return partial derivatives dy/du_i for all variables

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

- 1. Write an **algorithm** for evaluating the function y = f(**x**). The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation**
- **graph")**
Visit each node in **topological order.** 2. Visit each node in **topological order.**
For variable u_i with inputs v₁,..., v_N
	- a. Compute $u_i = g_i(v_1, ..., v_N)$
	- b. Store the result at the node

Backward Computation (Version B)

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

Backpropagation

Why is the backpropagation algorithm efficient?

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

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

Background

A Recipe for adients and the learning Gradients

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

2. Choose each of the

– Decision function

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

– Loss function

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

1. Given training dat **Backpropagation** can compute this gradient!

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

opposite the gradient)

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

MATRIX CALCULUS

Q&A

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

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

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

Numerator

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

> Denominator *Denominator*

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

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

1. In numerator layout:

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

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

2. In denominator layout:

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

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

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

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

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

DRAWING A NEURAL NETWORK

Ways of Drawing Neural Networks

Neural Network Diagram

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

Ways of Drawing Neural Networks

Computation Graph

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

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

Summary

- **1. Neural Networks**…
	- provide a way of learning features
	- are highly nonlinear prediction functions
	- (can be) a highly parallel network of logistic regression classifiers
	- discover useful hidden representations of the input

2. Backpropagation…

- provides an efficient way to compute gradients
- is a special case of reverse-mode automatic differentiation

Backprop Objectives

You should be able to…

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

DEEP LEARNING

Why is everyone talking about Deep Learning?

- Because a lot of money is invested in it…
	- DeepMind: Acquired by Google for **\$400 million**
	- Deep Learning startups command **millions of VC dollars**
	- Demand for deep learning engineers continually outpaces supply
- Because it made the **front page** of the New York Times

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Petuur

Why is everyone talking about Deep Learning?

Deep learning:

- Has won numerous pattern recognition competitions
- Does so with minimal feature engineering

This wasn't always the case! Since 1980s: Form of models hasn't changed much, but lots of new tricks…

- More hidden units
- Better (online) optimization
- New nonlinear functions (ReLUs)
- Faster computers (CPUs and GPUs)

FIRST EXAMPLE OF A DEEP NETWORK

To-601 course staff

BACKGROUND: HUMAN LANGUAGE TECHNOLOGIES

Human Language Technologies

Speech Recognition

Machine Translation

기계 번역은 특히 영어와 한국어와 같은 언어 쌍의 경우 매우 어렵습니다.

Summarization

Bidirectional RNN

RNNs are a now commonplace backbone in deep learning approaches to natural language processing

BACKGROUND: COMPUTER VISION

Example: Image Classification

- ImageNet LSVRC-2011 contest:
	- **Dataset**: 1.2 million labeled images, 1000 classes
	- **Task**: Given a new image, label it with the correct class
	- **Multiclass** classification problem
- Examples from http://image-net.org/

IMAGENET

Bird

Warm-blooded egg-laying vertebrates characterized by feathers and forelimbs modified as wings

2126

pictures

Popularity
Percentile

Not logged in. Login I Signup

92.85% Wordnet IDs

IMAGENET

14,197,122 images, 21841 synsets indexed

SEARCH

Explore Home About Download

Not logged in. Login I Signup

IMAGENET

SEARCH

 $Home$ Explore About Download

Not logged in. Login I Signup

Feature Engineering for CV

Edge detection (Canny)

Corner Detection (Harris) Scale Invariant Feature Transform (SIFT)

Figures from http://opencv.org

Figure from Lowe (1999) and Lowe (2004)

Example: Image Classification

CNN for Image Classification (Krizhevsky, Sutskever & Hinton, 2012) 15.3% error on ImageNet LSVRC-2012 contest

Input

image (pixels)

- Five convolutional layers (w/max-pooling)
- Three fully connected layers

1000-way

softmax

CNNs for Image Recognition

Backpropagation and Deep Learning

Convolutional neural networks (CNNs) and **recurrent neural networks** (RNNs) are simply fancy computation graphs (aka. hypotheses or decision functions).

Our recipe also applies to these models and (again) relies on the **backpropagation algorithm** to compute the necessary gradients.

BACKGROUND: N-GRAM LANGUAGE MODELS

- *Goal*: Generate realistic looking sentences in a human language
- *Key Idea*: condition on the last n-1 words to sample the n^{th} word

Learning an n-Gram Model

Question: How do we **learn** the probabilities for the n-Gram Model?

Learning an n-Gram Model

Question: How do we **learn** the probabilities for the n-Gram Model?

Answer: From data! Just **count** n-gram frequencies

- …the **cows eat grass**…
- …our **cows eat hay** daily…
- …factory-farm **cows eat corn**…
- …on an organic farm, **cows eat hay** and…
- …do your **cows eat grass** or corn?...
- …what do **cows eat if** they have…
- …**cows eat corn** when there is no…
- …which **cows eat which** foods depends…
- …if **cows eat grass**…
- …when **cows eat corn** their stomachs…
- …should we let **cows eat corn**?...

 $p(w_t | w_{t-2} = \text{cows},$ $w_{t-1} = eat)$

Sampling from a Language Model

Question: How do we sample from a Language Model?

Answer:

- 1. Treat each probability distribution like a (50k-sided) weighted die
- 2. Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$
- 3. Roll that die and generate whichever word w_t lands face up

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4. Repeat

RECURRENT NEURAL NETWORK (RNN) LANGUAGE MODELS

Recurrent Neural Networks (RNNs) $\left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array} \right)$ **h** $\left(\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array} \right)$ (*y*1*,...,y^T*) by iterating the following equations from *t* = 1

where the *W* terms denote weight matrices (e.g. *Wxh* is the $\textrm{inputs: } \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$ Definition of the RNN: hidden units: $\mathbf{h} = (h_1, h_2, \dots, h_T), h_i \in \mathcal{R}^J$ outputs: $\mathbf{y} = (y_1, y_2, \dots, y_T), y_i \in \mathcal{R}^K$ nonlinearity: *H*

Definition of the RNN:
\n
$$
h_t = \mathcal{H} (W_{xh} x_t + W_{hh} h_{t-1} + b_h)
$$
\n
$$
y_t = W_{hy} h_t + b_y
$$

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RNN Language Model

 T **RNN Language Model:** $p(w_1, w_2, \ldots, w_T) = \prod p(w_t | f_{\theta}(w_{t-1}, \ldots, w_1))$ $t=1$

Key Idea:

(1) convert all previous words to a **fixed length vector** (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector

RNN Language Model

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(1) convert all previous words to a **fixed length vector** (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector **¹¹⁸**

Key Idea:

 $p(w_1, w_2, w_3, ..., w_T) = p(w_1 | h_1) p(w_2 | h_2) ... p(w_2 | h_T)$

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- 3. Roll that die and generate whichever word w_t lands face up

Which is the real

Shakespeare?!

??

VIOLA: Why, Salisbury must find his flesh and thought That which I am not aps, not a man and in fire, To show the reining of the raven and the wars To grace my hand reproach within, and not a fair are hand, That Caesar and my goodly father's world; When I was heaven of presence and our fleets, We spare with hours, but cut thy

council I am great, Murdered a master's ready there My powe so much as hell: Some service i bondman here, Would show hi

KING LEAR: O, if you we reeble sight, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

??

CHARLES: Marry, do I, sir; and I came to acquaint you with a matter. I am given, sir, secretly to understand that your younger brother Orlando hath a disposition to come in disguised against me to try a fall. To-morrow, sir, I wrestle for my credit; and he that escapes me without some broken limb shall acquit him

is but young and tender; and, uld be loath to foil him, as I honour, if he come in:

therefore, one of the my love to you, I came hither
that either you might \sum_{α} that either you might stay him from his interior brown disgrace well as he shall run into, in that it is a thing of his own search and altogether against my will.

Shakespeare's As You Like It

VIOLA: Why, Salisbury must find his flesh and thought That which I am not aps, not a man and in fire, To show the reining of the raven and the wars To grace my hand reproach within, and not a fair are hand, That Caesar and my goodly father's world; When I was heaven of presence and our fleets, We spare with hours, but cut thy council I am great, Murdered and by thy master's ready there My power to give thee but so much as hell: Some service in the noble bondman here, Would show him to her wine.

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RNN-LM Sample

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SEQUENCE TO SEQUENCE MODELS

Sequence to Sequence Model

Speech Recognition

Machine Translation

기계 번역은 특히 영어와 한국어와 같은 언어 쌍의 경우 매우 어렵습니다.

Summarization

Sequence to Sequence Model

Now suppose you want generate a sequence conditioned on another input

Key Idea:

Encoder

- 1. Use an **encoder** model to generate a vector representation of the **input**
- 2. Feed the output of the encoder to a **decoder** which will generate the **output**

Applications:

- translation: Spanish \rightarrow English
- summarization: article \rightarrow summary
- speech recognition: speech signal \rightarrow transcription

