- This session is recorded.
- Mute your mic.
- You can leave messages in the chat panel to ask questions.
- When I check your progress, please click of if you are done.
- We will start at 6:35.

CS5242 Neural Networks and Deep Learning

Lecture 01: Introduction and Linear Regression

Wei WANG

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change log: V1: slide 41, the superscript should be n



Agenda

- Introduction of this module
 - Logistics
 - History
- Linear regression
 - Univariate
 - Multivariate

Instructor

- WANG Wei
 - COM2-04-09
 - wangwei@comp.nus.edu.sg

- Research
 - Machine learning system optimization
 - Multi-modal data analysis/applications

Teaching Assistants



LIANG Yuxuan
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Quiz



FU Di e0409760@u.nus.edu Assignment



FU Yujian
e0427770@u.nus.edu
Final project

Your background?

LumiNUS Poll

Pre-requisite

Course

- Machine Learning (CS3244)
 - Or https://www.coursera.org/learn/machine-learning
- Linear Algebra (MA1101R)
 - Or https://ocw.mit.edu/courses/mathematics/18-06-linear-algebra-spring-2010/
- Calculus (MA1521)
- Probability (ST2334)
- Brief summary

Coding

- Python (ONLY, version 3.x)
 - Numpy
 - Keras, TensorFlow, PyTorch, MxNet, Caffe, SINGA
- Jupyter notebook or Google colab

Grading policy

Weightage:

- Assignment 30 points
- Two assignments
- 15% off per day late (17:01 is the start of one day); 0 score if you submit it 7 days after the deadline
- Online quiz 30 points
- 3 quizzes in total
- You need a camera (from your laptop, mobile phone or external camera)
- Project 40 points
- Kaggle competition
- Group size <=4

Collaboration

- Every assignment is an individual task
- The project is a group-based task
- Avoid academic offence (cheating, plagiarism including copying code from the internet, e.g., github)

Contacts

- LumiNUS forum
 - For all issues
- Email: cs5242@comp.nus.edu.sg
 - For private/personal issues
- Consultation (make appointments on LumiNUS)
 - Wei WANG, wangwei@comp.nus.edu.sg
 - Wed, 11:00-12:00

GPU machines

- SoC GPU machines
 - https://dochub.comp.nus.edu.sg/cf/guides/compute-cluster/hardware
- Google Cloud Platform
 - Some free credit for new register
 - GPU is expensive
- Amazon EC2 (g2.8xlarge)
 - Some free credit for students
 - GPU is expensive
- NSCC (National Super-Computing Center)
 - Free for NUS students
 - The libraries are sometimes outdated
 - Jobs will be submitted into a queue for executing
- Important notes if you use cloud platforms:
 - STOP/TERMINATE the instance immediately after your program terminates
 - Check the usage status frequently to avoid high outstanding bills
 - Amazon/Google may charge you for additional storage volume

Syllabus & Schedule

- Learn various neural network models
 - From shallow to deep neural networks
 - Including the model structure, training algorithms, tricks and applications
 - Covering the principles, coding practices and a bit theory
- Check LumiNUS for the latest plan

Intended learning outcomes (my expectation)

1

Explain the principles of the operations of different layers and training algorithms

2

Compare different neural network architectures

3

Implement popular neural networks

4

Solve problems using neural networks and deep learning techniques

Your expectation?

I want to get an easy boost to my GPA.

This course may not be easy

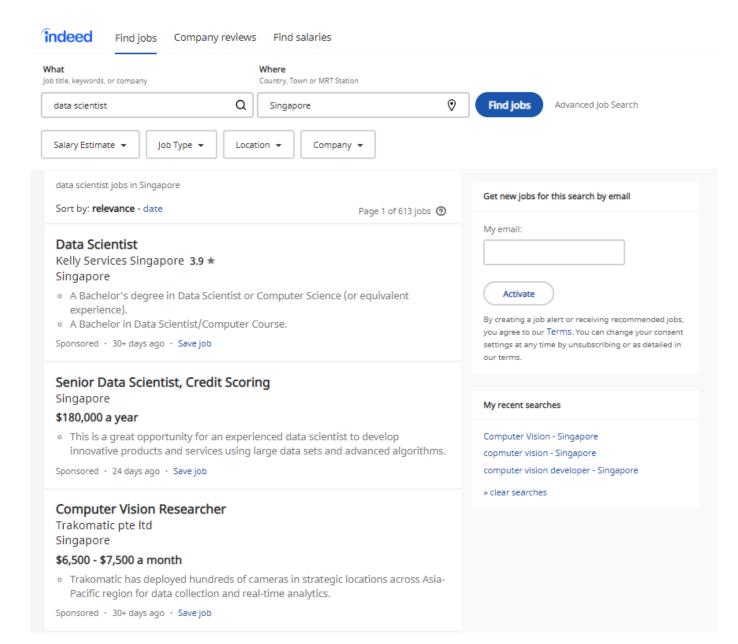
I want to earn the big bucks as a data scientist / ML engineer at Google / Amazon / Facebook.



This course provides the basics; but is not enough.

check out:

CS5260 - NN & Deep Learning II CS4243 - Computer Vision & Pattern Recognition CS4248 - Natural Language Processing





My PhD advisor is making me take this course so that I can use deep learning in our research.

Neural Networks and Deep Learning:

- Andrew Ng
- https://www.coursera.org/learn/neural-networks-deep-learning

CSC 321: Intro to Neural Networks and Machine Learning

- Roger Grosse
- http://www.cs.toronto.edu/~rgrosse/courses/csc321 2017/

Neural Networks for Machine Learning

- Geoffrey Hinton
- https://www.coursera.org/learn/neural-networks

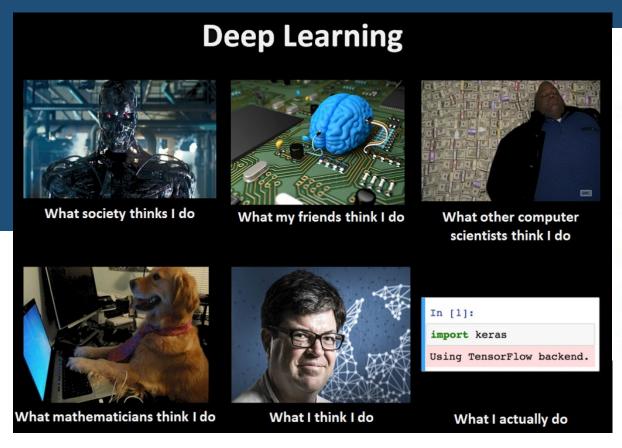
CS231n: Convolutional Neural Networks for Visual Recognition

- Fei-Fei Li, Justin Johnson, Serena Yeung
- http://cs231n.stanford.edu/

CS224d: Deep Learning for Natural Language Processing

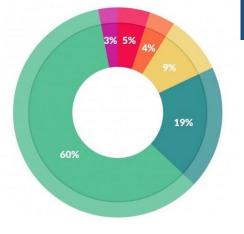
- Richard Socher
- http://cs224d.stanford.edu/

Al is cool and I want to build the next Skynet.

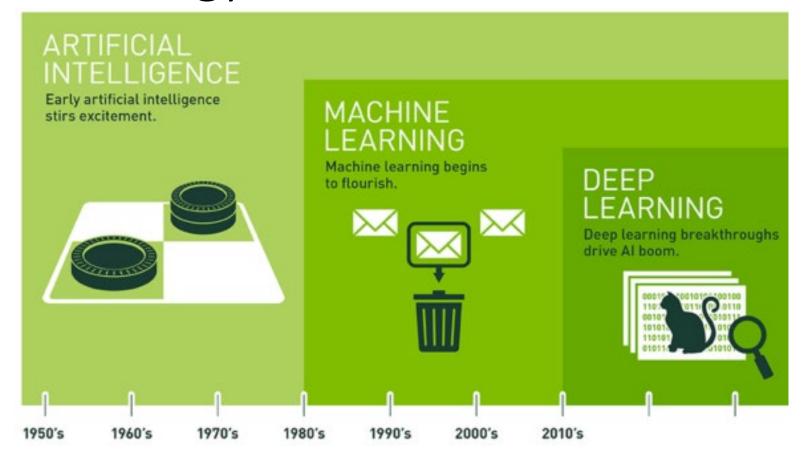


What data scientists spend the most time doing

- Building training sets: 3%
- Cleaning and organizing data: 60%
- Collecting data sets; 19%
- Mining data for patterns: 9%
- Refining algorithms: 4%
- Other: 5%



Terminology Overload: Al vs. ML vs. DL



Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

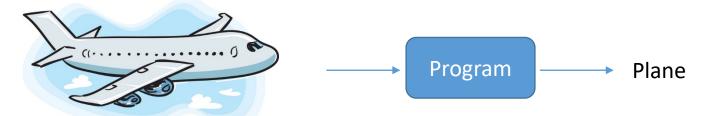
Al

- 1950's
- "Human intelligence exhibited by machines"
 - Expert systems; Rules
 - Machine learning algorithms
- Narrow AI: image recognition, machine translation

https://www.youtube.com/watch?v=nASDYRkbQIY

Machine Learning

- 1980's
- "An approach to achieve AI through systems that can learn from experience to find patterns in that data"
 - Can we code a program with rules (like bubble sorting) to do
 - Image recognition

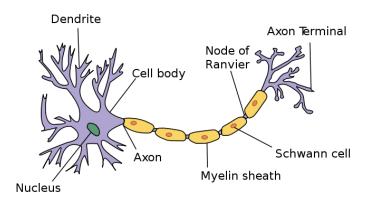


Speech recognition

<u>This Photo</u> by Unknown Author is licensed under CC BY-NC-ND

Neural networks and Deep Learning

- 1950's
- A class of machine learning algorithm that use a cascade of multiple layers of nonlinear processing units for feature extraction and transformation---Wikipedia



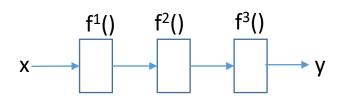
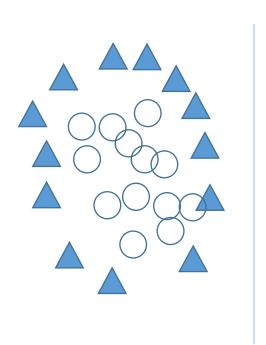


Image source: http://pediaa.com/difference-between-nerve-and-neuron/

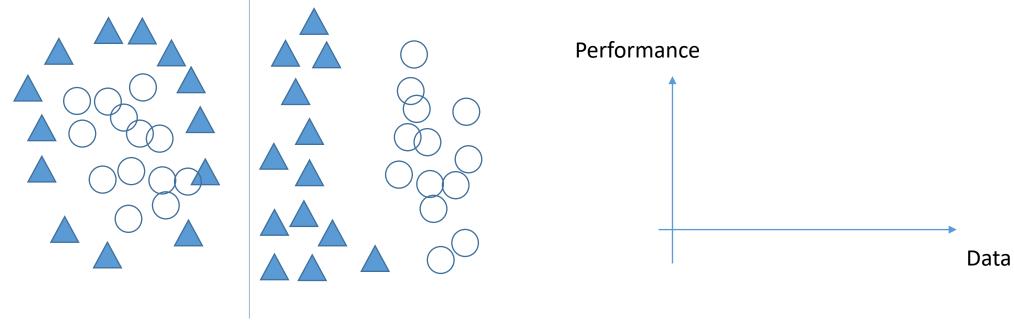
Neural networks and Deep Learning

Feature learning (transformation)



Neural networks and Deep Learning

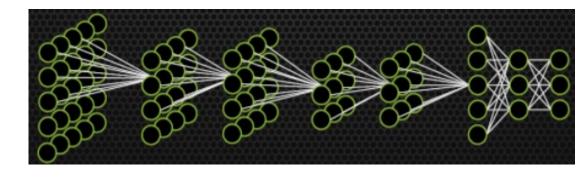
Feature learning (transformation)



Deep learning is not a killer for everything

Neural networks (NN)

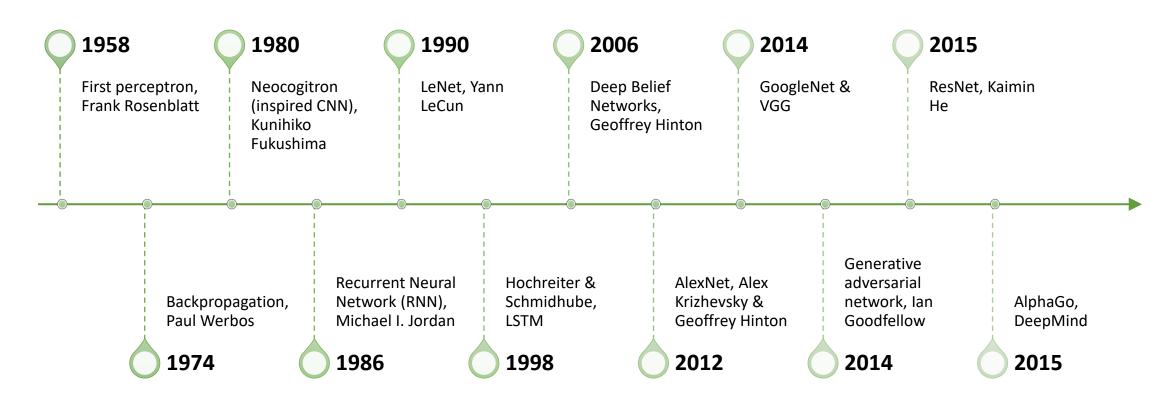
- Linear, polynomial, logistic, multinomial regression
- Perceptron and multi-layer perceptron (MLP)
- Convolutional neural network (CNN)
- Recurrent neural networks (RNN)
- Generative adversarial networks (GAN)
- (Restricted) Boltzmann machine
- Deep belief network
- Spike neural network
- Radial basis function neural network
- Hopfield networks



Source from [3]

History [2]

https://www.youtube.com/watch?v=yaL5ZMvRRqE



Refer to http://people.idsia.ch/~juergen/who-invented-backpropagation.html for more papers

Applications

Computer Vision

- <u>Image classification</u>
- Object detection, demo
- Scene text recognition
- Neural style transferring
- <u>Image generation</u>

Natural language processing

- Question answering
- Machine translation

Speech

• Speech recognition, e.g. <u>Amazon Echo</u>

Univariate Linear Regression

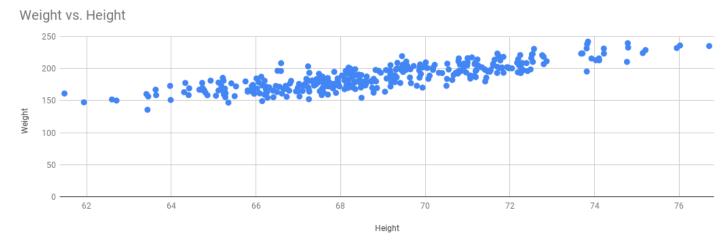
Weight vs Height

Problem definition:

• Predict the weight given the height of a person.

Data

- Input: Height (inches)
- Output: Weight (pounds)
- Split the data into
 - 80% for training
 - 20% for evaluation



Data source: https://www.kaggle.com/mustafaali96/weight-height

Modeling

- Notation
 - A person is called an example/instance
 - Height denoted as $x \in R$: input feature
 - Weight denoted as $y \in R$: the target or ground truth
- Map from input to output by linear regression
 - $\tilde{y} = xw + b, w \in R, b \in R$
 - w is the slope and b is the intercept
 - \tilde{y} is called the **prediction**

Training

- Learn w and b to fit the training data $S_{train} = \{(x^{(i)}, y^{(i)})\}, i = 1 \dots m$
 - That fit the data well
 - How to measure the quality of w and b?
- Loss function
 - The smaller the loss value, the better the prediction (closer to the target)
 - $L(x, y|w, b) = |\tilde{y} y|$
 - $L(x,y|w,b) = \frac{1}{2}||\tilde{y} y||^2 = \frac{1}{2}(\tilde{y} y)^2$
 - Easier for optimization/training because it is differentiable
 - The coefficient $\frac{1}{2}$ is to make the gradient simple
- Define the training objective
 - $J(w,b) = \frac{1}{m} \sum_{i=1}^{m} L(x^{(i)}, y^{(i)} | w, b)$

Optimization/training

Tune the model parameters over the training instances to minimize the average loss, i.e., the training objective

$$\min_{w,b} J(w,b)$$

$$\rightarrow \min_{w,b} \frac{1}{m} \sum_{i=1}^{m} L(x^{(i)}, y^{(i)} | w, b)$$

$$\to \min_{w,b} \frac{1}{2m} \sum_{i=1}^{m} (wx^{(i)} + b - y^{(i)})^2$$

Optimization/training

1. Fix b and learn w

$$\min_{w} \frac{1}{2m} \sum_{i=1}^{m} (x^{(i)})^{2} w^{2} + \frac{1}{m} \sum_{i=1}^{m} x^{(i)} (b - y^{(i)}) w + \frac{1}{2m} \sum_{i=1}^{m} (b - y^{(i)})^{2}$$

$$\rightarrow \min_{w} c_1 w^2 + c_2 w + c_3$$

2. Fix w and learn b

Gradient for univariate simple functions

Gradient: recall high school calculus and how to take derivatives

•
$$\frac{\partial f(x)}{\partial x} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

•
$$f(x) = 3, \frac{\partial f(x)}{\partial x} = 0$$

•
$$f(x) = 3x, \frac{\partial f(x)}{\partial x} = 3$$

•
$$f(x) = x^2$$
, $\frac{\partial f(x)}{\partial x} = 2x$

Gradient for univariate composite functions

•
$$f(x) = g(x) + h(x)$$

•
$$f(x) = 3x + x^2$$

•
$$f(x) = g(x)h(x)$$

• $f(x) = xx^2$

•
$$f(x) = \frac{g(x)}{h(x)}$$

• $f(x) = \frac{e^x}{x}$

•
$$f(x) = g(u), u = h(x)$$

• $f(x) = \ln(x + x^2)$

$$\bullet \ f'(x) = g'(x) + h'(x)$$

We use f'(x) and $\frac{\partial f(x)}{\partial x}$ interchangeably for the gradient of f(x) with respect to x, where x and f(x) are scalars

•
$$f'(x) = g'(x)h(x) + g(x)h'(x)$$

•
$$f'(x) = \frac{g'(x)h(x) - g(x)h'(x)}{h(x)^2}$$

•
$$f'(x) = g'(u)h'(x)$$

HW1: solve for the derivatives / gradients of these functions.

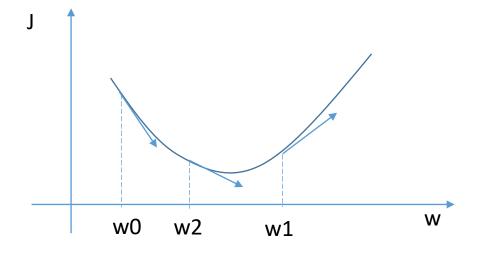
Training by gradient descent

$$J = c_1 w^2 + c_2 w + c_3$$

Find the w for which we have the lowest* J.

For example:

$$c_1 = 1, c_2 = -2, c_3 = 1$$



α is the learning rate, which controls the moving step length. It's important for convergence. If it is large, w oscillates around the optimal position. If it is small, it takes many iterations to reach the optimum.

Initialize w as w0 Compute $\frac{\partial J}{\partial w}|_{w=w0}$, negative; Move w from w0 to the right by $w1=w0+\alpha\frac{\partial J}{\partial w}|_{w=w0}$



Compute $\frac{\partial J}{\partial w}|_{w=w1}$, positive; Move w from w1 to the left by $w2 = w1 - \alpha \frac{\partial J}{\partial w}|_{w=w1}$



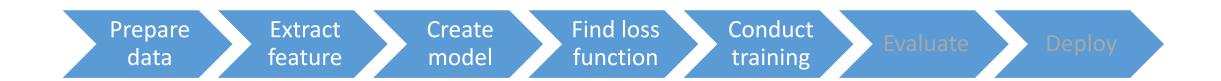
Compute $\frac{\partial J}{\partial w}|_{w=w2}$, negative Move w from w2 to the right by w3 = w2 + $\alpha \frac{\partial J}{\partial w}|_{w=w2}$

Training by gradient descent

- Gradient descent algorithm for optimization
- Set w = 0.1 or a random number
- Repeat
 - For each data sample, compute $\tilde{y} = xw + b$
 - Compute the average loss, $\sum_{\langle x,y \rangle \in S_{train}} L(x,y|w,b) / |S_{train}|$
 - Compute $\frac{\partial J}{\partial w}$
 - Update $w = w \alpha \frac{\partial J}{\partial w}$

Update w, b repeatedly...
What if there are multiple parameters, e.g., multiple variables?

Machine learning pipeline



Multivariate Linear Regression

Multivariate linear regression

- Consider the problem of <u>house price prediction</u>
- Each instance in the training dataset
 - Denote the features using a column vector
 - $x \in R^{n \times 1}$: x_i is the i-th feature
 - size, floor, location, age, lease, etc.
 - Target $y \in R$: price

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$$

Model

Map from input to output

$$\tilde{y} = w^T x + b$$
, $w \in R^{n \times 1}$, $b \in R$, w_i is the i-th element of w (importance of i-th feature)

$$=\sum_{i=1}^{n}w_{i}x_{i}+b$$
 The summation is over n elements, where n is the number of features per instance.

$$= (w_1, w_2, \dots, w_n) \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} + b$$

=
$$(w_1, w_2, ..., w_n, b)$$
 $\begin{pmatrix} x_1 \\ x_2 \\ ... \\ x_n \\ 1 \end{pmatrix}$

$$\rightarrow \tilde{y} = \overline{\boldsymbol{w}}^T \overline{\boldsymbol{x}}$$

For the rest of this module, we use w and x for \overline{w} and \overline{x} respectively unless there is a special definition of w and x.

Optimization

- Compute the gradient of the loss with respect to (w.r.t) w
 - Consider a single instance

$$J(\mathbf{w}) = L \ (\mathbf{x}, \mathbf{y} | \mathbf{w}) = \frac{1}{2} ||\tilde{\mathbf{y}} - \mathbf{y}||^2 = \frac{1}{2} (\mathbf{w}^T \mathbf{x} - \mathbf{y})^2$$

$$\frac{\partial J(w)}{\partial w} = ?$$

Gradient of vector and matrix (denominator layout)

- Vectors
 - By default, is a column vector
 - Denoted as x, y, z

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{bmatrix} \qquad \frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} & \frac{\partial y_2}{\partial x} & \dots & \frac{\partial y_m}{\partial x} \end{bmatrix}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix}
\frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\
\frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_2} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial y_1}{\partial x_n} & \frac{\partial y_2}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n}
\end{bmatrix}.$$

Denominator layout: the result shape is (n, m)

Gradient of vector and matrix (denominator layout)

- Matrix
 - Denoted as X, Y, Z

$$\frac{\partial \mathbf{Y}}{\partial x} = \begin{bmatrix} \frac{\partial y_{11}}{\partial x} & \frac{\partial y_{21}}{\partial x} & \dots & \frac{\partial y_{m1}}{\partial x} \\ \frac{\partial y_{12}}{\partial x} & \frac{\partial y_{22}}{\partial x} & \dots & \frac{\partial y_{m2}}{\partial x} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_{1n}}{\partial x} & \frac{\partial y_{2n}}{\partial x} & \dots & \frac{\partial y_{mn}}{\partial x} \end{bmatrix}$$

$$\frac{\partial y}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial y}{\partial x_{11}} & \frac{\partial y}{\partial x_{12}} & \cdots & \frac{\partial y}{\partial x_{1q}} \\ \frac{\partial y}{\partial x_{21}} & \frac{\partial y}{\partial x_{22}} & \cdots & \frac{\partial y}{\partial x_{2q}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial x_{p1}} & \frac{\partial y}{\partial x_{p2}} & \cdots & \frac{\partial y}{\partial x_{pq}} \end{bmatrix}$$

Gradient of matrix with respect to (w.r.t) matrix, matrix w.r.t vector, vector w.r.t matrix?

Too complex. Not commonly used.

Gradient table

(denominator layout)

Shape of $\frac{\partial y}{\partial x}$	Scalar y	Vector y (m ,1)	Matrix Y (m, n)
Scalar x	?	?	?
Vector x (n,1)	(n, 1)	?	
Matrix X (p, q)	?		

HW2: fill in the table with the matrix dimensions of the resulting gradients.

Gradient table: vector by vector (denominator layout)

HW3: fill in the gradient table with the resulting gradients

y =	а	x	Ax	$x^T A$
$\frac{\partial y}{\partial x} =$?	?	A^T	Ş

<i>y</i> =	$\begin{array}{c c} a\mathbf{u} \\ \mathbf{u} = \mathbf{u}(\mathbf{x}) \end{array}$	$vu \\ v = v(x), u = u(x)$	v + u $v = v(x), u = u(x)$	$Au \\ u = u(x)$	$g(\mathbf{u})$ $\mathbf{u} = \mathbf{u}(\mathbf{x})$
$\frac{\partial y}{\partial x} =$?	$v\frac{\partial u}{\partial x} + \frac{\partial v}{\partial x}u^T$?	?	?

y =	а	$ \begin{array}{c c} u^T v \\ v = v(x), u = u(x) \end{array} $	g(u) $u = u(x)$	$x^T A x$
$\frac{\partial y}{\partial x} =$?	?	?	?

Optimization

- Compute the gradient of the loss w.r.t w
 - Consider a single instance

$$J(\mathbf{w}) = L \ (\mathbf{x}, \mathbf{y} | \mathbf{w}) = \frac{1}{2} || \tilde{\mathbf{y}} - \mathbf{y} ||^2 = \frac{1}{2} (\mathbf{w}^T \mathbf{x} - \mathbf{y})^2$$

$$\frac{\partial J(w)}{\partial w} = ?$$

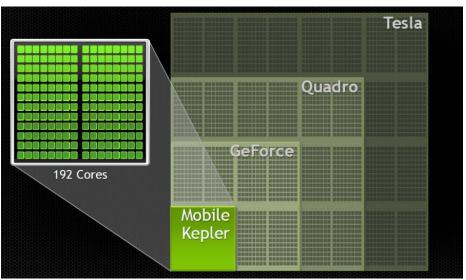
$$z = \mathbf{w}^{T} \mathbf{x} - \mathbf{y}$$

$$J(\mathbf{w}) = \frac{1}{2} z^{2}$$

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = \frac{\partial J}{\partial z} \frac{\partial z}{\partial \mathbf{w}} = z\mathbf{x} = (\mathbf{w}^{T} \mathbf{x} - \mathbf{y})\mathbf{x}$$

Shape Check!

- Consider multiple examples $\{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}$, i=1, 2, ..., m
- Naïve approach of computing the gradient
 - for each instance $(x^{(i)}, y^{(i)})$
 - Accumulate the loss $L(x^{(i)}, y^{(i)})$ into J
 - Average J over m
 - for each instance $(x^{(i)}, y^{(i)})$
 - Accumulate the gradient of $\frac{\partial L(x^{(i)}, y^{(i)})}{\partial w}$
- Not as fast as matrix operations



- Consider multiple examples $\{(x^{(i)}, y^{(i)})\}$, i=1, 2, ..., m
- Put each instance (the feature vector) into one row of a matrix
 - For fast memory access as Numpy stores data in row-major format
- Put each target into one element of a column vector

• Put each target into one element of a column
$$X = \begin{pmatrix} x^{(1)^T} \\ x^{(2)^T} \\ \dots \\ x^{(m)^T} \end{pmatrix}$$
 $y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \dots \\ y^{(m)} \end{pmatrix}$ $\widetilde{y} = Xw$

$$J(w) = ?$$

- Consider multiple examples $\{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}$, i=1, 2, ..., m
- Put each instance (the feature vector) into one row of a matrix
 - For fast memory access as Numpy stores data in row-major format
- Put each target into one element of a column vector

$$X = \begin{pmatrix} \mathbf{x}^{(1)^T} \\ \mathbf{x}^{(2)^T} \\ \dots \\ \mathbf{x}^{(m)^T} \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} \mathbf{y}^{(1)} \\ \mathbf{y}^{(2)} \\ \dots \\ \mathbf{y}^{(m)} \end{pmatrix}$$

$$J(\mathbf{w}) = \frac{1}{2m} ||\widetilde{\mathbf{y}} - \mathbf{y}||^2 = \frac{1}{2m} (\widetilde{\mathbf{y}} - \mathbf{y})^{\mathrm{T}} (\widetilde{\mathbf{y}} - \mathbf{y}) \qquad \mathbf{u} = \widetilde{\mathbf{y}} - \mathbf{y}$$

$$\partial J(\mathbf{w})$$

$$\frac{\partial f(w)}{\partial w} = 2$$

- Consider multiple examples $\{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}$, i=1, 2, ..., m
- Put each instance (the feature vector) into one row of a matrix
 - For fast memory access as numpy stores data in row-major format
- Put each target into one element of a column vector

$$X = \begin{pmatrix} x^{(1)^T} \\ x^{(2)^T} \\ \dots \\ x^{(m)^T} \end{pmatrix} \qquad y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \dots \\ y^{(m)} \end{pmatrix}$$

$$J(w) = \frac{1}{2m} ||\widetilde{y} - y||^2 = \frac{1}{2m} (\widetilde{y} - y)^T (\widetilde{y} - y) \qquad u = \widetilde{y} - y$$

$$\frac{\partial J(w)}{\partial w} = \frac{1}{2m} \left(\frac{\partial u}{\partial w} u + \frac{\partial u}{\partial w} u \right) = \frac{1}{m} X^T u = \frac{1}{m} X^T (\widetilde{y} - y) \qquad \text{Shape Check!}$$

Training by gradient descent

- Gradient descent algorithm for optimization
- initialize w randomly
- Repeat
 - Compute the objective I(w) over all training instances

 - Compute $\frac{\partial J}{\partial w}$ Update $\mathbf{w} = \mathbf{w} \alpha \frac{\partial J}{\partial w}$

Notation summary

- Scalar x
- Vector $x \in \mathbb{R}^{n \times 1}$
 - i-th element of a vector, x_i
 - i-th example $x^{(i)}$
- Matrix X
 - i-th row and j-th column X_{ij}
- If we choose denominator layout for $\frac{\partial y}{\partial x}$ we should lay out the gradient $\frac{\partial y}{\partial x}$ as a column vector, and $\frac{\partial y}{\partial x}$ as a row vector.

Summary

- Al vs. ML vs. Deep Learning
- Terminologies & Notations
 - Feature, label, loss
- Univariate & multivariate linear regression
 - Solving parameters via gradient descent
 - Taking gradients of vectors & matrices

References

- [1] Goodfellow Ian, Bengio Yoshua, Courville Aaron. Deep learning. MIT Press. http://www.deeplearningbook.org
- [2] Haohan Wang, Bhiksha Raj. On the Origin of Deep Learning. 2017 https://arxiv.org/abs/1702.07800
- [3] H. Lee, R. Grosse, R. Ranganath, and A. Y. Ng. "Convolutional deep belief networks for scalable unsupervised learning of hierarchical representations." In ICML 2009
- http://neuralnetworksanddeeplearning.com/chap1.html
- https://www.analyticsvidhya.com/blog/2017/06/a-comprehensive-guide-for-linear-ridge-and-lasso-regression/
- https://medium.com/meta-design-ideas/math-stats-and-nlp-for-machine-learning-as-fast-as-possible-915ef47ced5f

Homework

Theory

- 1. Solve for the gradients of the functions. (slide 34)
- 2. Solve for the dimensionality of the gradient vectors (slide 44)
- 3. Fill out the gradient tables (slide 45).

<u>Practical</u>

1. https://tinyurl.com/y26qj2ts

Next Lecture

(Shallow) Neural Networks