Today's Lecture

- 1. Get to know each other
 - Instructor & TAs
 - Students
- 2. Module Introduction
- 3. Logistics
- 4. Linear Regression

Let's get to know each other.

If you cannot come to the classroom

1. Join Zoom Meeting https://nus-sg.zoom.us/j/3997998157

2. Meeting ID: 399 799 8157

I heard that everyone got A's last term and am hoping for an easy boost to my GPA.

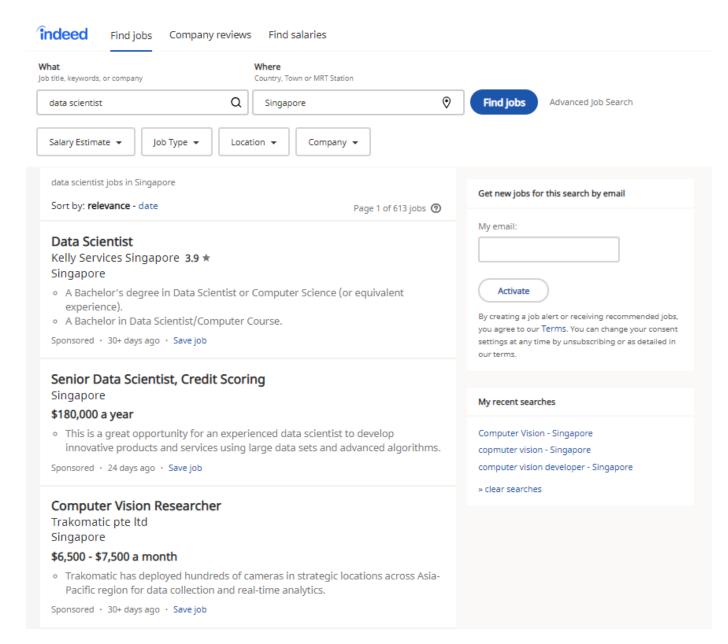
maybe, maybe not...

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



checkout

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





I actually wanted CS5XXX but couldn't get that module.

too bad 20

Can't get into this module? Email for guest access.

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

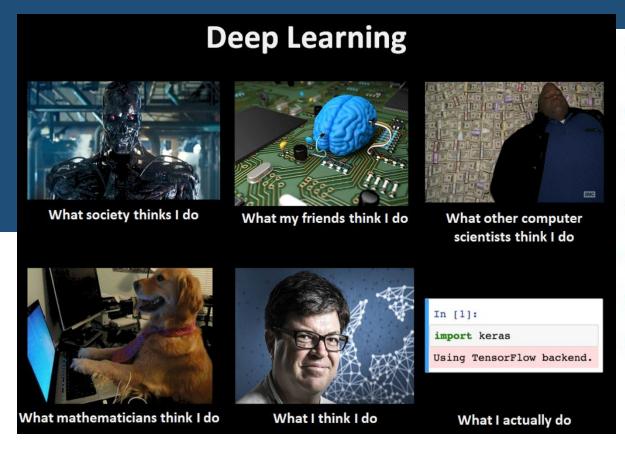
CS231n: Convolutional Neural Networks for Visual Recognition

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

CS224d: Deep Learning for Natural Language Processing

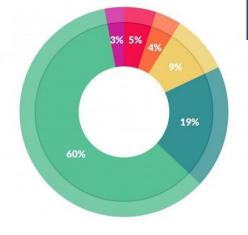
- Richard Socher
- http://cs224d.stanford.edu/

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%



Intended Learning Outcomes

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

Course Logistics

Pre-requisite

Modules

- 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, Colossal-AI
- Jupyter notebook

Syllabus & Schedule

- Learn various neural network models
 - From shallow to deep neural networks
 - model structures, training algorithms, tricks and applications
 - principles, theory & coding practices
- Check Canvas (not LumiNUS) for the latest plan
 - https://canvas.nus.edu.sg/

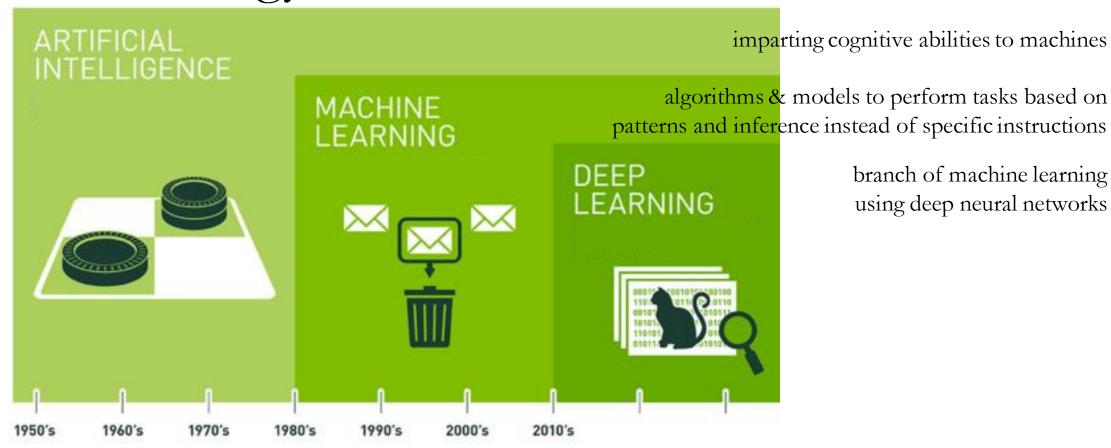
GPU machines

- SoC GPU machines:
 - https://dochub.comp.nus.edu.sg/cf/guides/compute-cluster/hardware
- NSCC (National Super-Computing Center)
 - Free for NUS students
 - The libraries are sometimes outdated
 - Jobs will be submitted into a queue for executing
- Google Cloud Platform
 - Some free credit for new register
 - GPU is expensive
- Amazon EC2 (g2.8xlarge)
 - Some free credit for students
 - GPU is expensive

Important notes if you use cloud platforms:

- STOP/TERMINATE the instance immediately after your program terminates
- Check usage status frequently to avoid high outstanding bills
- Amazon/Google may charge you for additional storage volume

Terminology Overload: AI vs. ML vs. DL

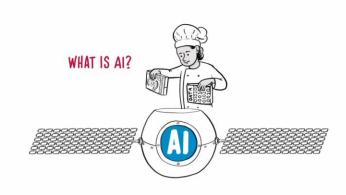


branch of machine learning using deep neural networks

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.

Artificial Intelligence (AI)

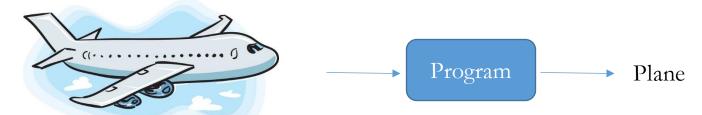
- 1950's
- "Human intelligence exhibited by machines"
 - Expert systems; Rules
 - Machine learning algorithms
- Narrow AI:
 - image recognition
 - machine translation
 - recommender system
 - . . .



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

Machine Learning (ML)

- 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 to do
 - Image recognition

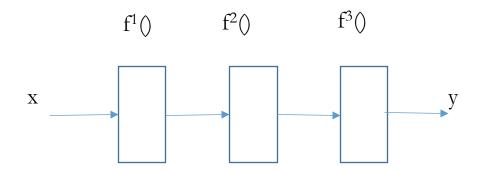


• Speech recognition

This Photo by Unknown Author is licensed under CC BY-NC-ND

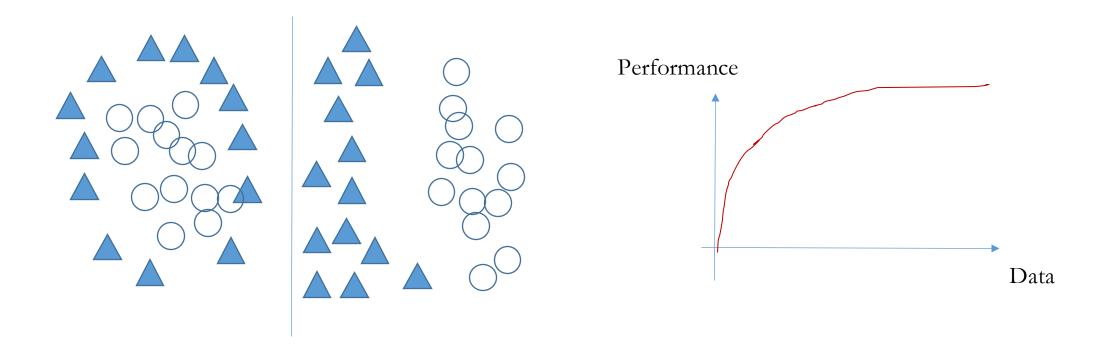
Neural networks and Deep Learning

- 1950's / 2010's



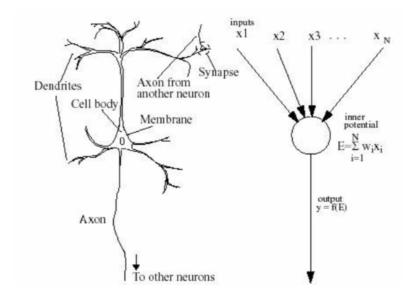
Neural networks and Deep Learning

• Feature learning (transformation)



"Neural" Networks?

The origins of neural networks come from efforts of mathematically representing information processing in biological systems (hence the term "neural").



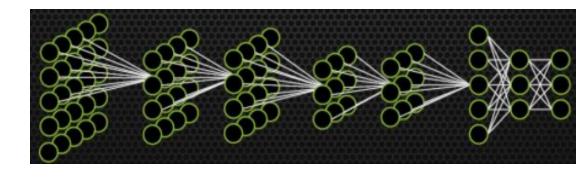
Neural nets/perceptrons are loosely inspired by biology. But they certainly are not a model of how the brain works, or even how neurons work.

http://commonsenseatheism.com/wp-content/uploads/2011/12/biological-and-artificial-neurons.jpg

Our interests in neural networks are less about biological systems and more about efficient models for statistical pattern recognition.

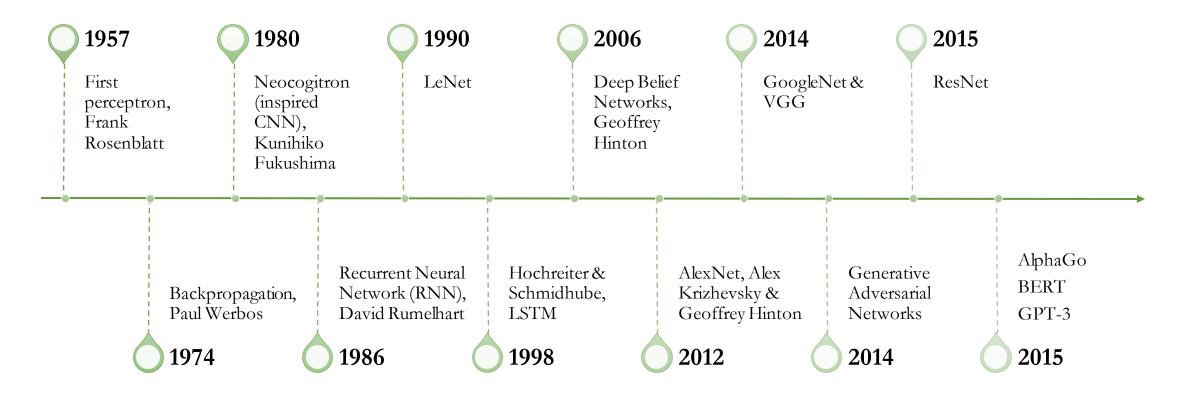
Neural networks (NN)

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



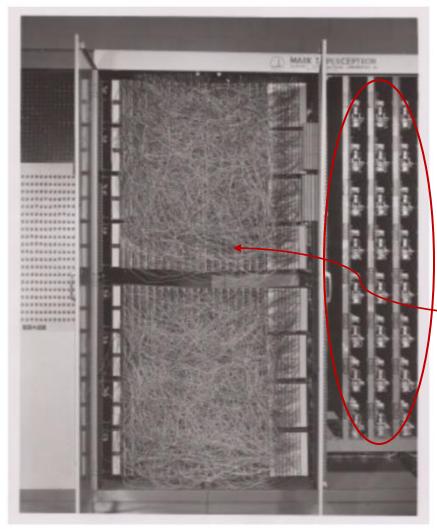
Source from [3]

History [2]



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

The Perceptron Machine (1957)

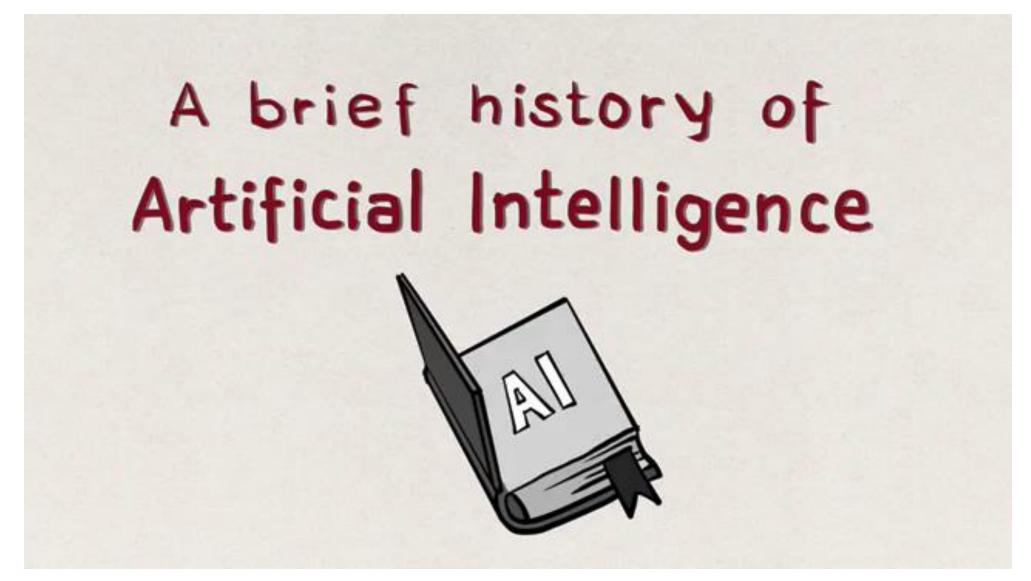


The Mark I Perceptron machine was a hardware implementation of the perceptron algorithm.

The Perceptron machine was connected to a 20x20 array of photocells producing a 400 pixel image (essentially a camera).

The nest of wires create different combinations of inputs.

Arrays of adjustable variable resistors, which could be used as adaptive ("hand-tuned") weights.



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

Applications

Computer Vision

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

Natural language processing

- Question answering
- Machine translation

Speech

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

Univariate Linear Regression

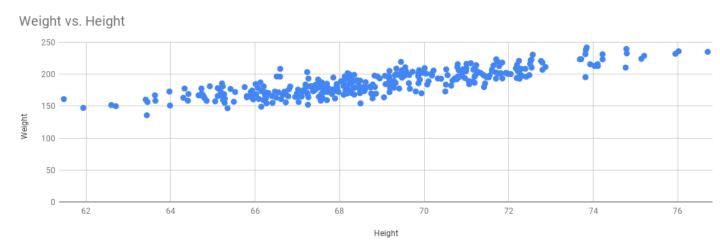
Weight vs Height

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
 - 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

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

Optimization/training

Fix b and learn w

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

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

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 simple functions

• Subgradient for non-differentiable points

•
$$f(x) = |x|, \frac{\partial f(x)}{\partial x} = \begin{cases} 1, for \ x > 0 \\ -1, for \ x < 0 \\ a \in [-1, 1], for \ x = 0 \end{cases}$$

Sign of the variable if it's non-zero, anything in [−1, 1] if it's zero.

•
$$f(x) = \max(x, 0)$$
, $\frac{\partial f(x)}{\partial x} = \begin{cases} 1, & \text{for } x > 0 \\ 0, & \text{for } x < 0 \\ a \in [0, 1], & \text{for } x = 0 \end{cases}$

Gradient for univariate composite functions

•
$$f(x) = g(x) + h(x)$$

• $f(x) = 3x + x^2$

•
$$f(x) = g(x)h(x)$$

• $f(x) = xx^2$

•
$$f(x) = \frac{g(x)}{h(x)}$$

• $f(x) = \frac{e^x}{x}$

•
$$f(x) = g(u), u = h(x)$$

• $f(x) = \ln(x + x^2)$

•
$$f'(x) = g'(x) + h'(x)$$
 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

•
$$f'(x) = g'(x)h(x) + g(x)h'(x)$$

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

•
$$f'(x) = g'(u)h'(x)$$

Training by gradient descent

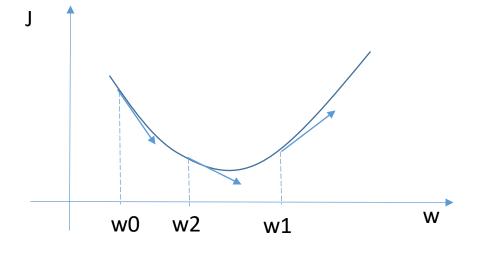
$$J(w)pprox w^2c_1+wc_2+c_3$$

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
$$\frac{\partial J}{\partial w} \mid_{w=w0}$$
, negative;
Move w from w0 to the right by

$$w1 = w0 \left(-\alpha \frac{\partial J}{\partial w} \right)_{w=w0}$$



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 $\hat{y} = xw + b$
 - 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...

Machine learning pipeline



Multivariate Linear Regression

Multivariate linear regression

- Consider the problem of house price prediction
- Each instance in the training dataset
 - Denote the features using a column vector

•
$$x \in \mathbb{R}^{n \times 1}$$
: x_i is the i-th feature

- size, floor, location, age, lease, etc.
- Target $y \in R$: price

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

<u>Model</u>

• Map from input to output $y = w^T x + b, w \in R^{n \times 1}, b \in R$, w_i is the i-th element of w (importance of i-th feature) $= \sum_{i=1}^m w_i x_i + b$ $= (w_1, w_2, \dots, w_n) \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} + b$ $= (w_1, w_2, \dots, w_n, b) \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$

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

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{bmatrix} \quad \frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} & \frac{\partial y_2}{\partial x} & \cdots \\ \vdots & \vdots & \vdots \\ \frac{\partial y}{\partial x_n} & \frac{\partial y_n}{\partial x_n} & \cdots \end{bmatrix}$$
Denominator layout: the

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

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

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.

Optimization

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

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

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

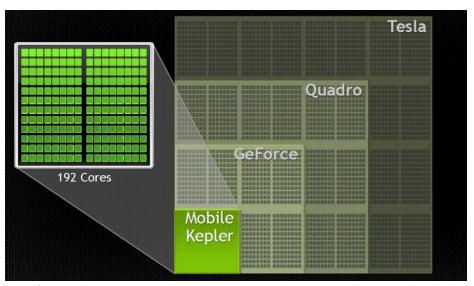
$$z = \mathbf{w}^T \mathbf{x} - \mathbf{y}$$

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

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

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 $\{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}$, 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 <u>row-major format</u>
- Put each target into one element of a column vector

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

$$J(w) = ?$$

- 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 <u>row-major format</u>
- Put each target into one element of a column vector

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

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

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

- 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 <u>row-major format</u>
- Put each target into one element of a column vector

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

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

$$\frac{\partial J(w)}{\partial w} = \frac{1}{2m} \left(\frac{\partial u}{\partial w} u + \frac{\partial u}{\partial w} u \right) = \frac{1}{m} X^T u = \frac{1}{m} X^T (y - y)$$

Training by gradient descent

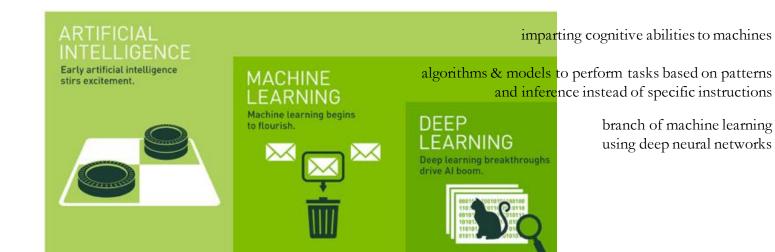
- Gradient descent algorithm for optimization
- initialize **w** randomly
- Repeat
 - Compute the objective J(w) over all training instances
 - Compute $\frac{\partial J}{\partial w}$
 - Update $\mathbf{w} = \mathbf{w} \alpha \frac{\partial J}{\partial w}$

Notation summary

- Scalar *x*
- Vector $\mathbf{x} \in \mathbb{R}^{n \times 1}$
 - 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.

<u>Summary</u>

• AI vs. ML vs. Deep Learning



- Taking gradients of vectors & matrices
- Univariate & multivariate linear regression
 - Updating parameters via gradient descent

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

TAs will let you know soon

Next Lecture

(Shallow) Neural Networks