Machine Learning Basics

Deep Learning & NLP for Computational Chemistry, Biology & Nano-materials

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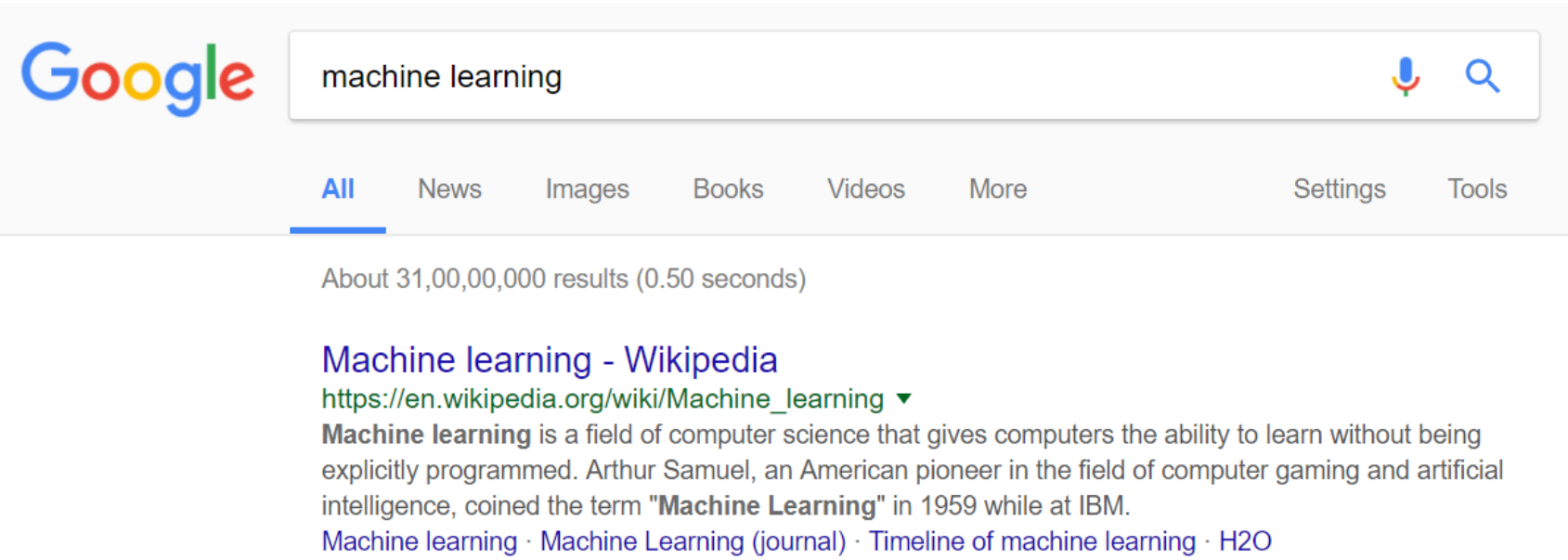
Outline

Machine Learning


Google
machine learning
All
News
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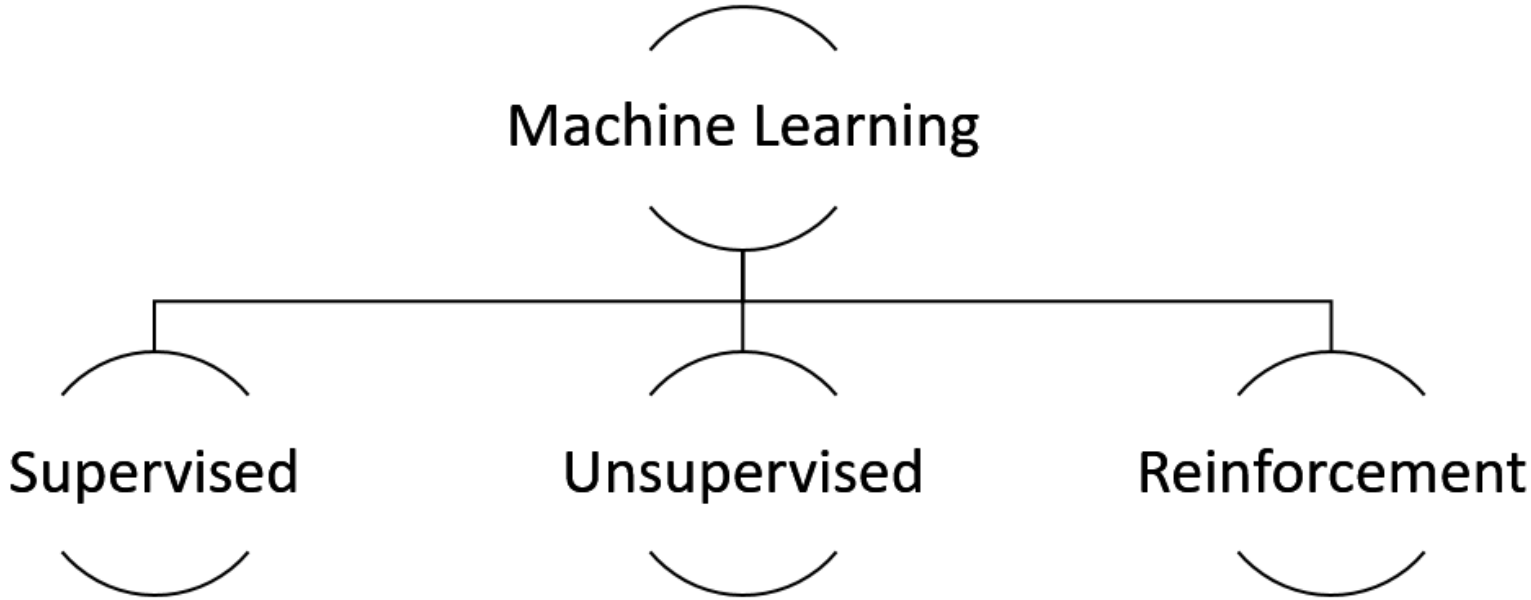
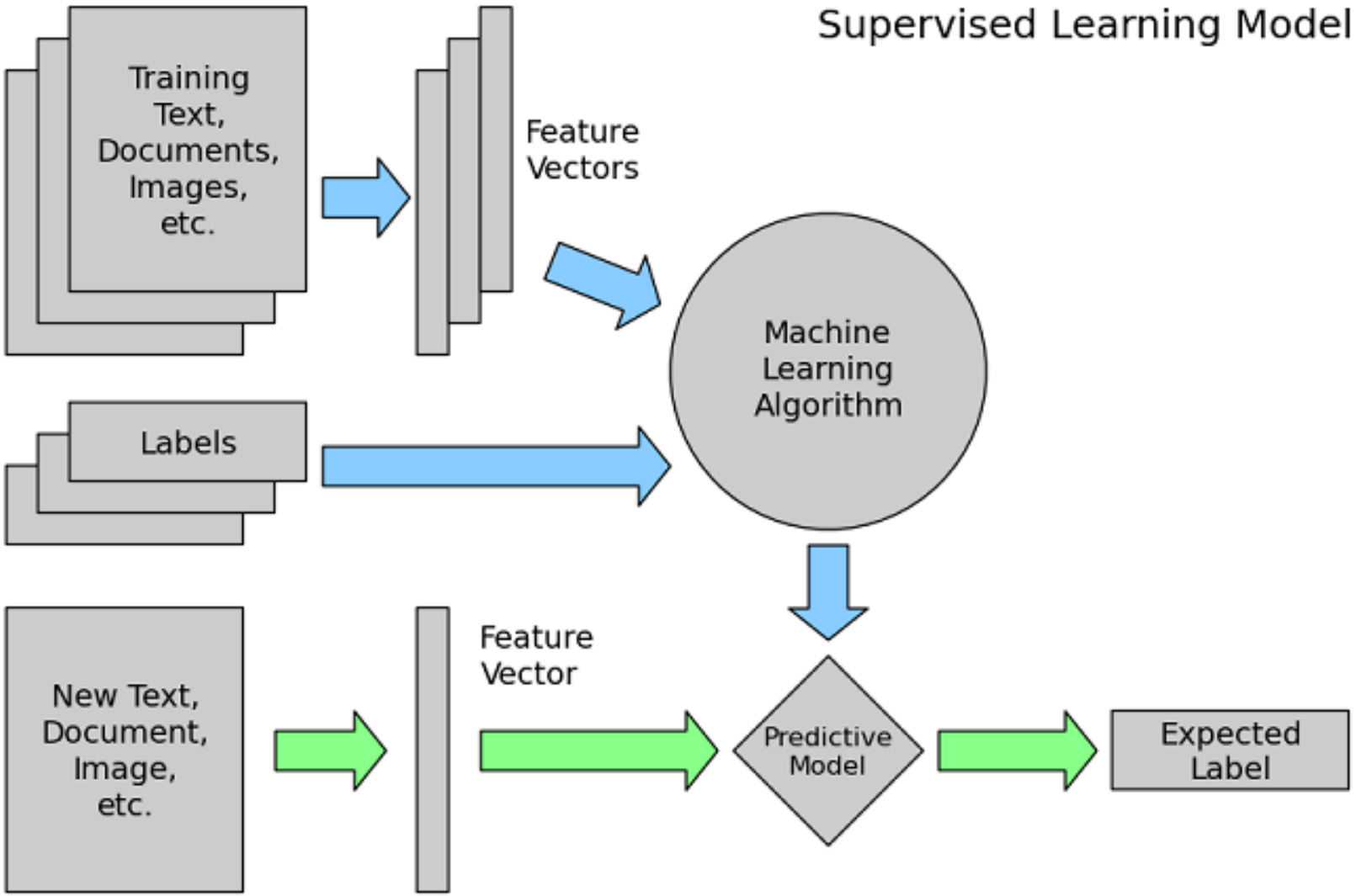
Books
Videos
More
Settings
Tools
About 31,00,00,000 results (0.50 seconds)
Machine learning - Wikipedia
https://en.wikipedia.org/wiki/Machine_learning
Machine learning is a field of computer science that gives computers the ability to learn without being explicitly programmed. Arthur Samuel, an American pioneer in the field of computer gaming and artificial intelligence, coined the term "Machine Learning" in 1959 while at IBM.
Machine learning · Machine Learning (journal) · Timeline of machine learning · H2O

- Reducing human/machine efforts required to perform a task (time optimization).
- Increasing the performance of a task (efficiency optimization).

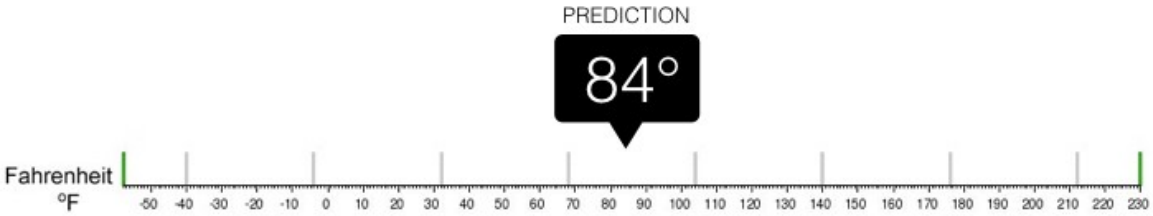

Machine Learning
Supervised
Unsupervised
Reinforcement



source: www.allprogrammingtutorials.com/tutorials/introduction-to-machine-learning.php

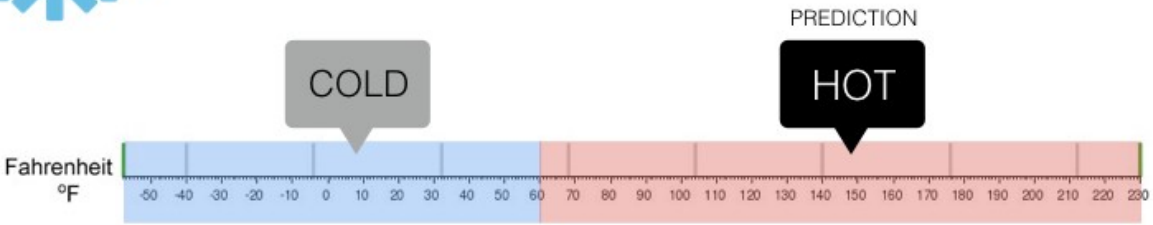
Regression

What is the temperature going to be tomorrow?



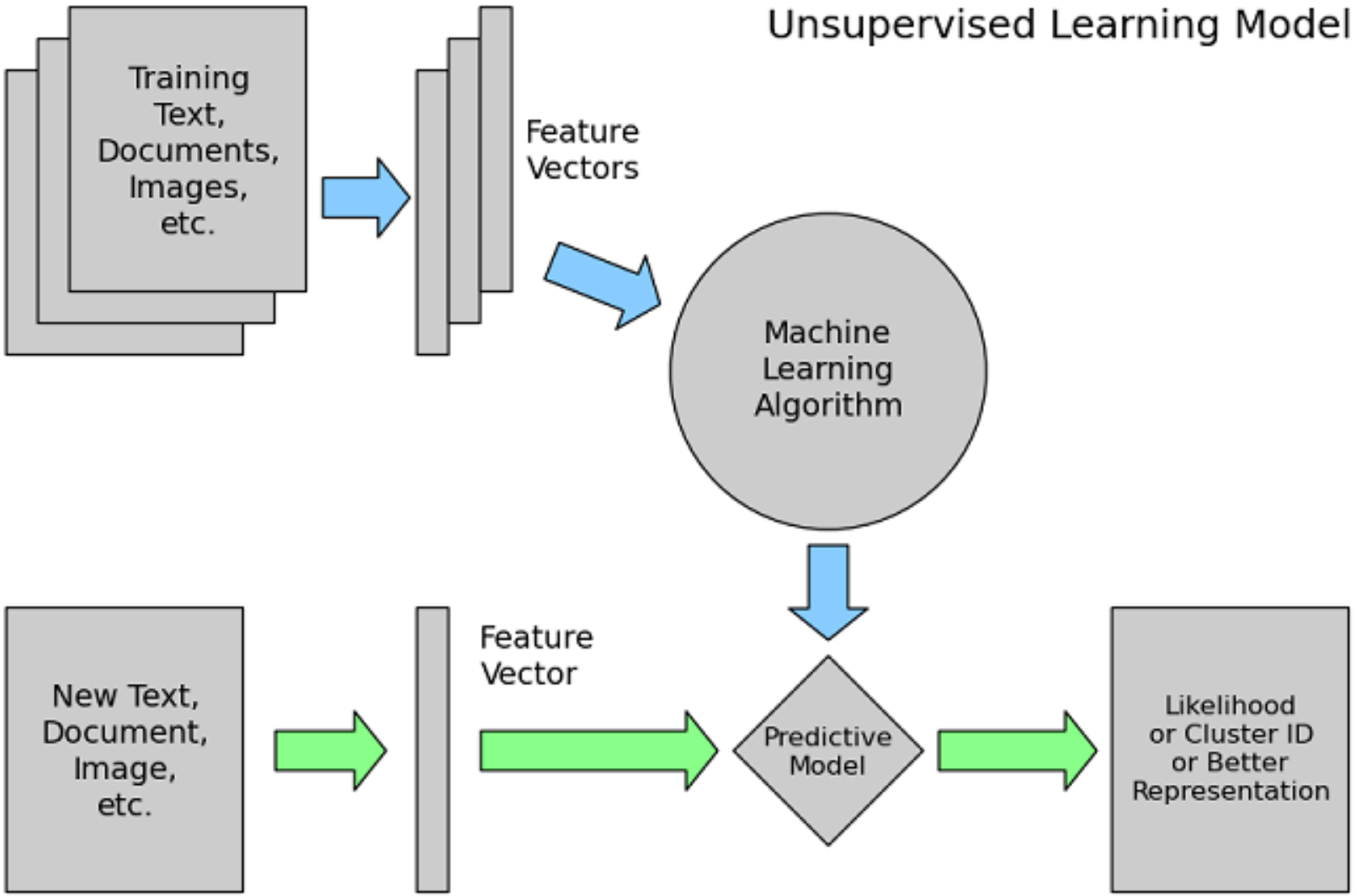
Classification

Will it be Cold or Hot tomorrow?



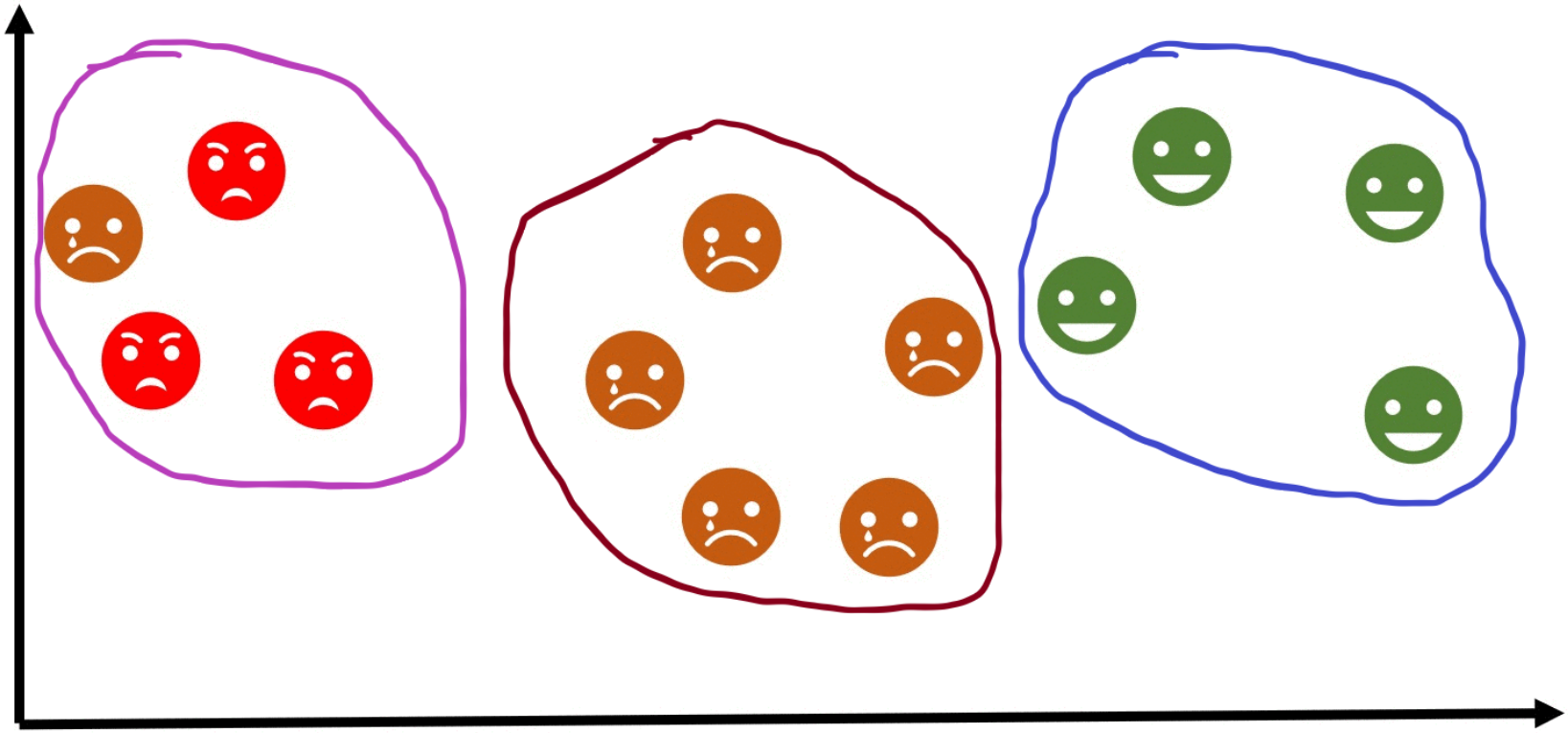
Common Supervised Learning Algorithms

- Decision Trees
- Support Vector Machines
- Support Vector Regression
- Linear Regression
- Logistic Regression
- Random Forest Tree



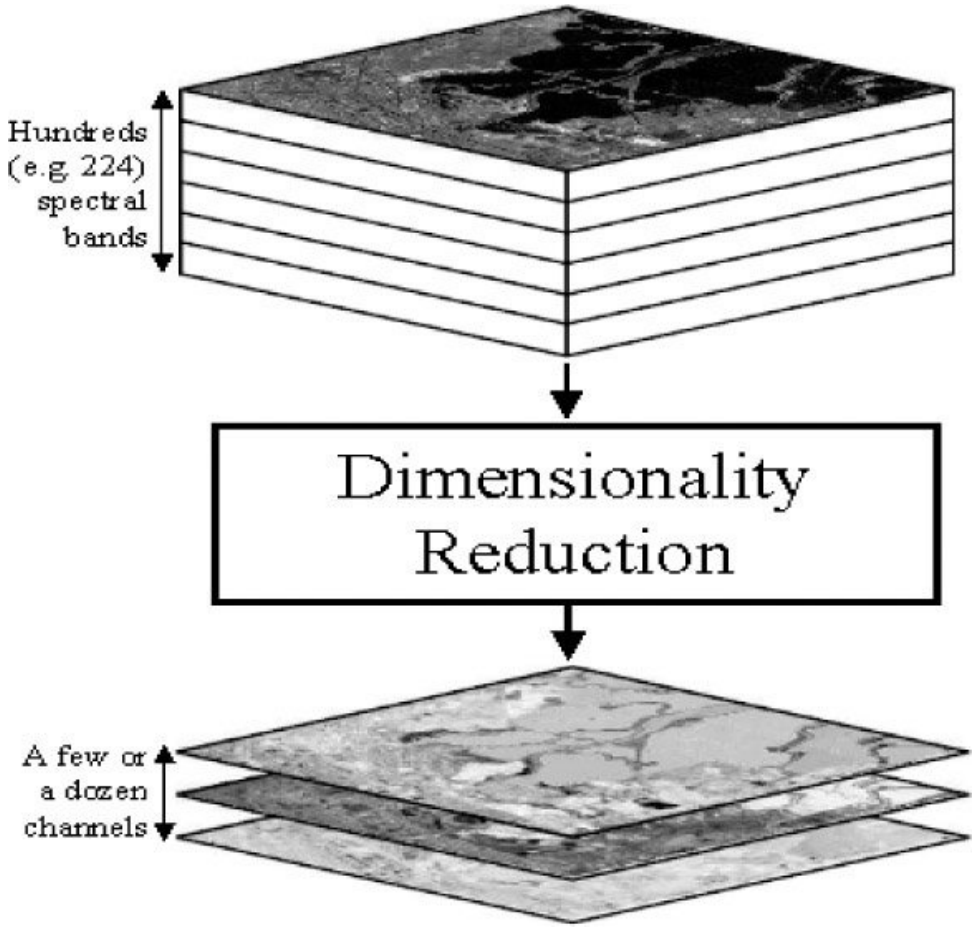
source: www.allprogrammingtutorials.com/tutorials/introduction-to-machine-learning.php

Clustering



source: https://towardsdatascience.com/clustering-unsupervised-learning-788b215b074b

Dimensionality Reduction

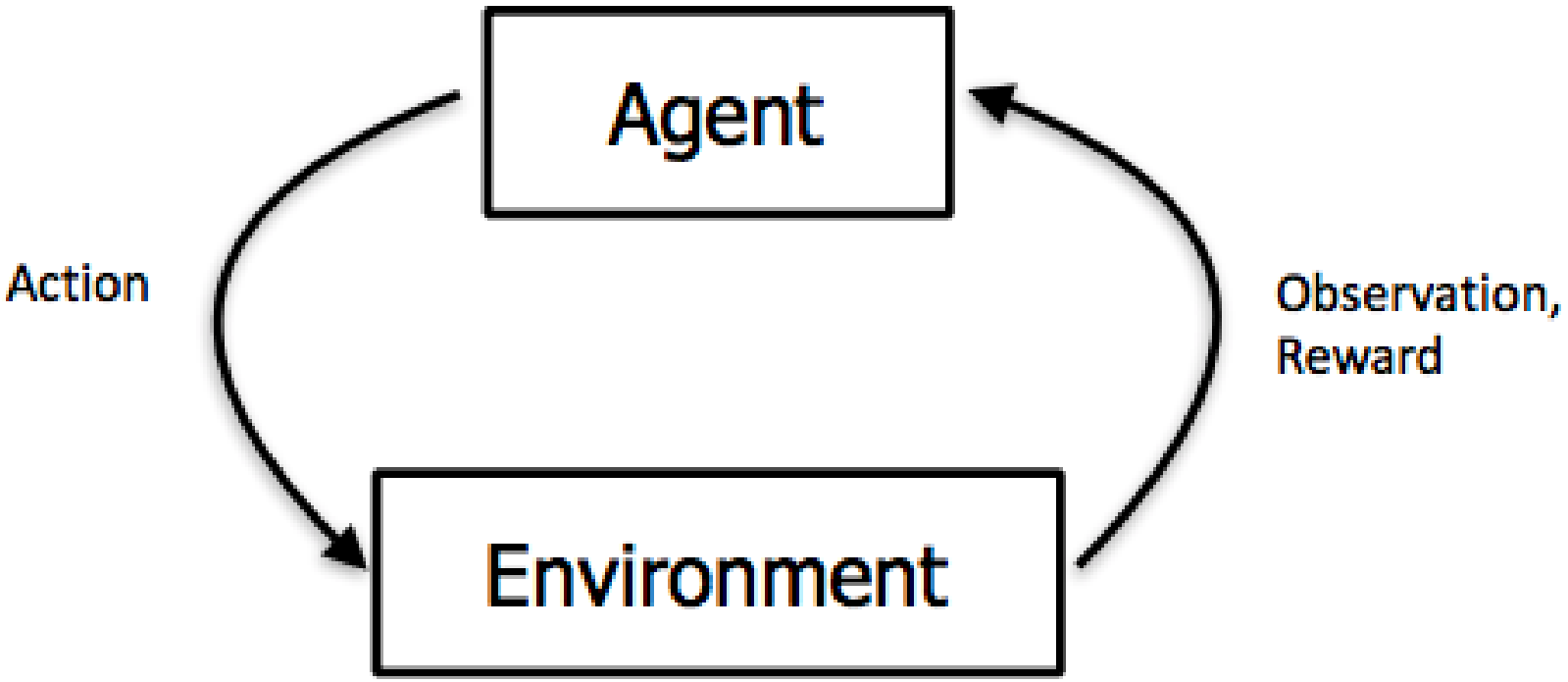


source: http://spie.org/newsroom/3560-dimensionality-reduction-of-multidimensional-satellite-imagery?SSO=1

Common Unsupervised Learning Algorithms

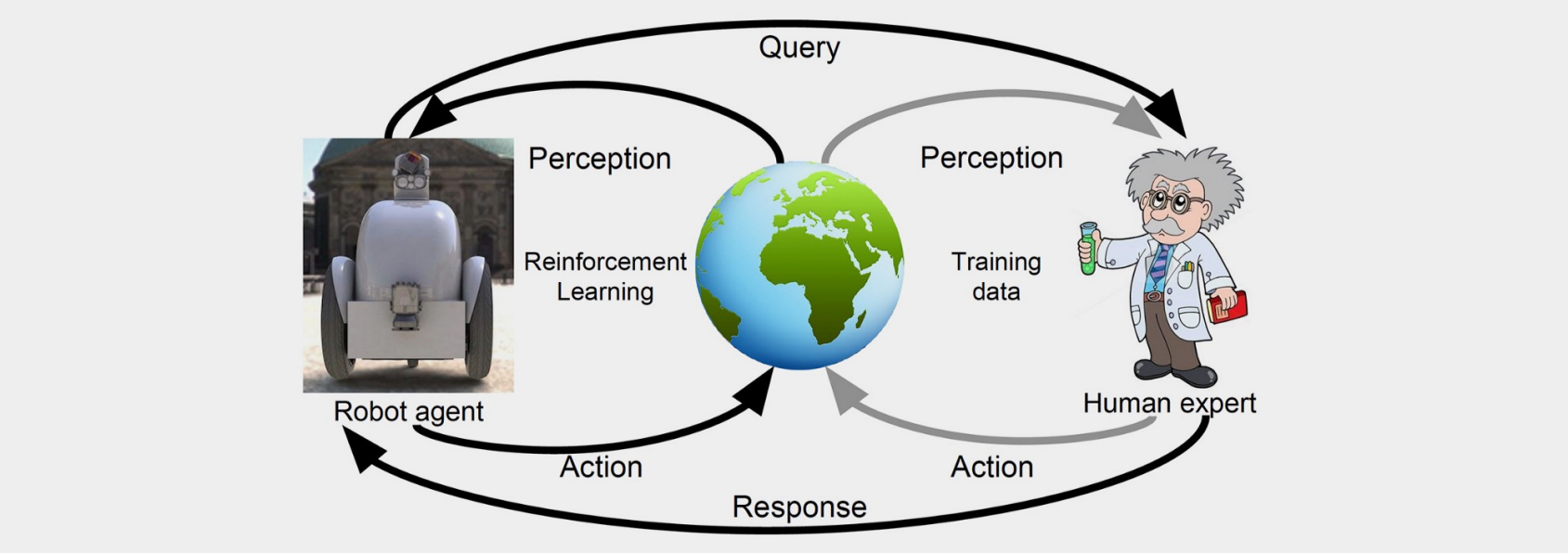
- K-means
- Affinity Propagation
- Hierarchical clustering
- Singluar Value Decomposition
- Latent Dirichlet Allocation
- Non-negative matrix factorization

Reinforcement Learning



source: https://medium.com/machine-learning-for-humans/reinforcement-learning-6eacf258b265

Reinforcement Learning



source:
https://chatbotsmagazine.com/reinforcement-learning-and-its-practical-applications-8499e60cf751

Common Reinforcement Learning Algorithms

- Q-Learning
- Temporal Difference (TD)
- Deep Adversarial Networks

DeepChem 2017

Rs. 300/- has to be paid for refreshment and materials at registration counter on the same date of workshop. (Excludes Food and Accommodation)

* Required

Full Name *

Your answer

Course *

- ○ BTech
- ○ Mtech
- ○ M.Sc
- ○ Ph.D
- ○ Other:

- Full Name
- Course
- Email
- Affiliation
- Contact No
- Phone number
- College Address

Matrix Representation

Linear Equations to Matrix

$$2a + b + c = 4 \tag{1}$$

$$a + 3b + 2c = 5 \tag{2}$$

$$a = 6 \tag{3}$$

Linear Equations to Matrix

$$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \tag{4}$$

Linear Equations to Matrix

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix}, \mathbf{x} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \quad (5)$$

Text to Matrix

- **S1:** We are in CEN.
- **S2:** CEN is in Amrita.
- **S3:** Amrita is in CBE.

Text to Matrix

- **S1:** We are in CEN.
- **S2:** CEN is in Amrita.
- **S3:** Amrita is in CBE.

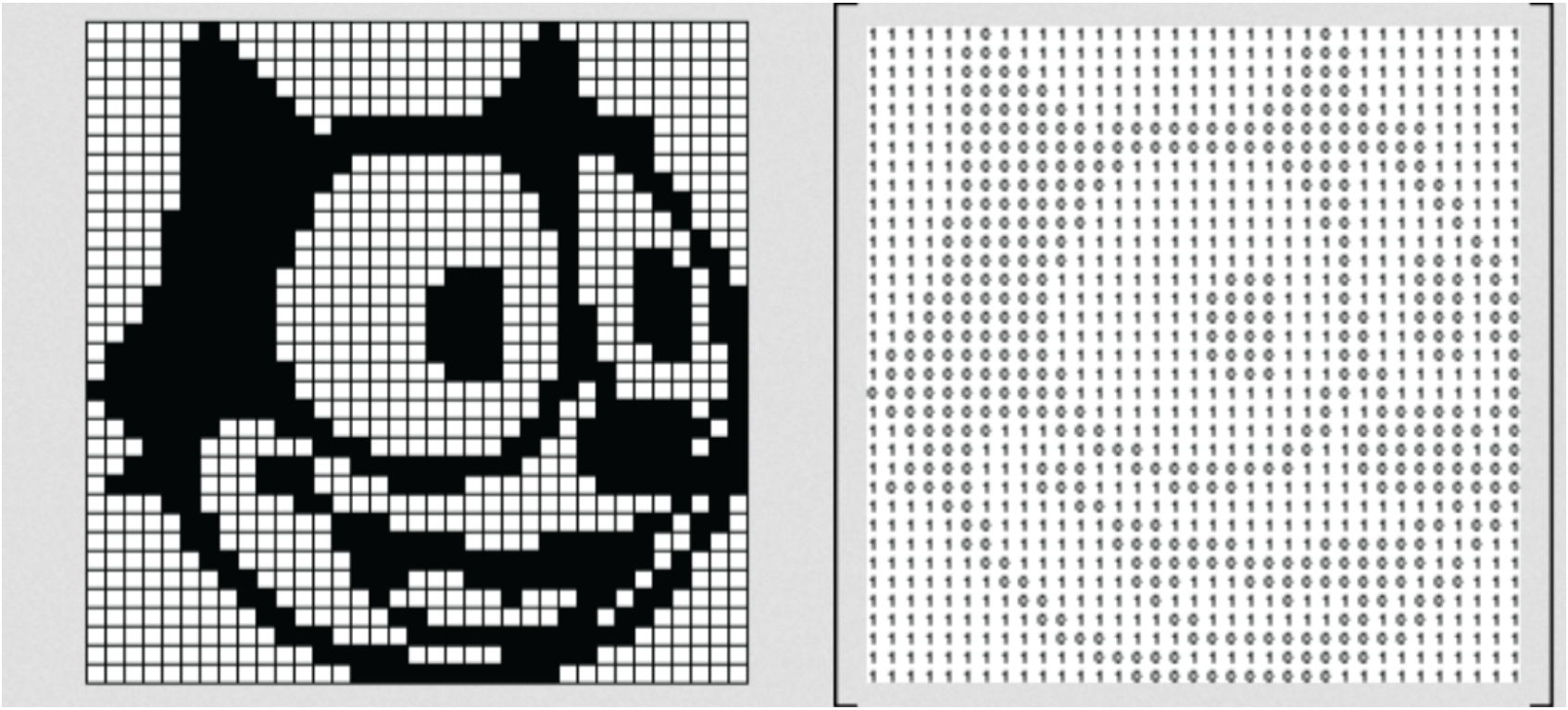
Vocabulary = amrita, are, cen, cbe, in, is, we

Text to Matrix

Table: Text Representation

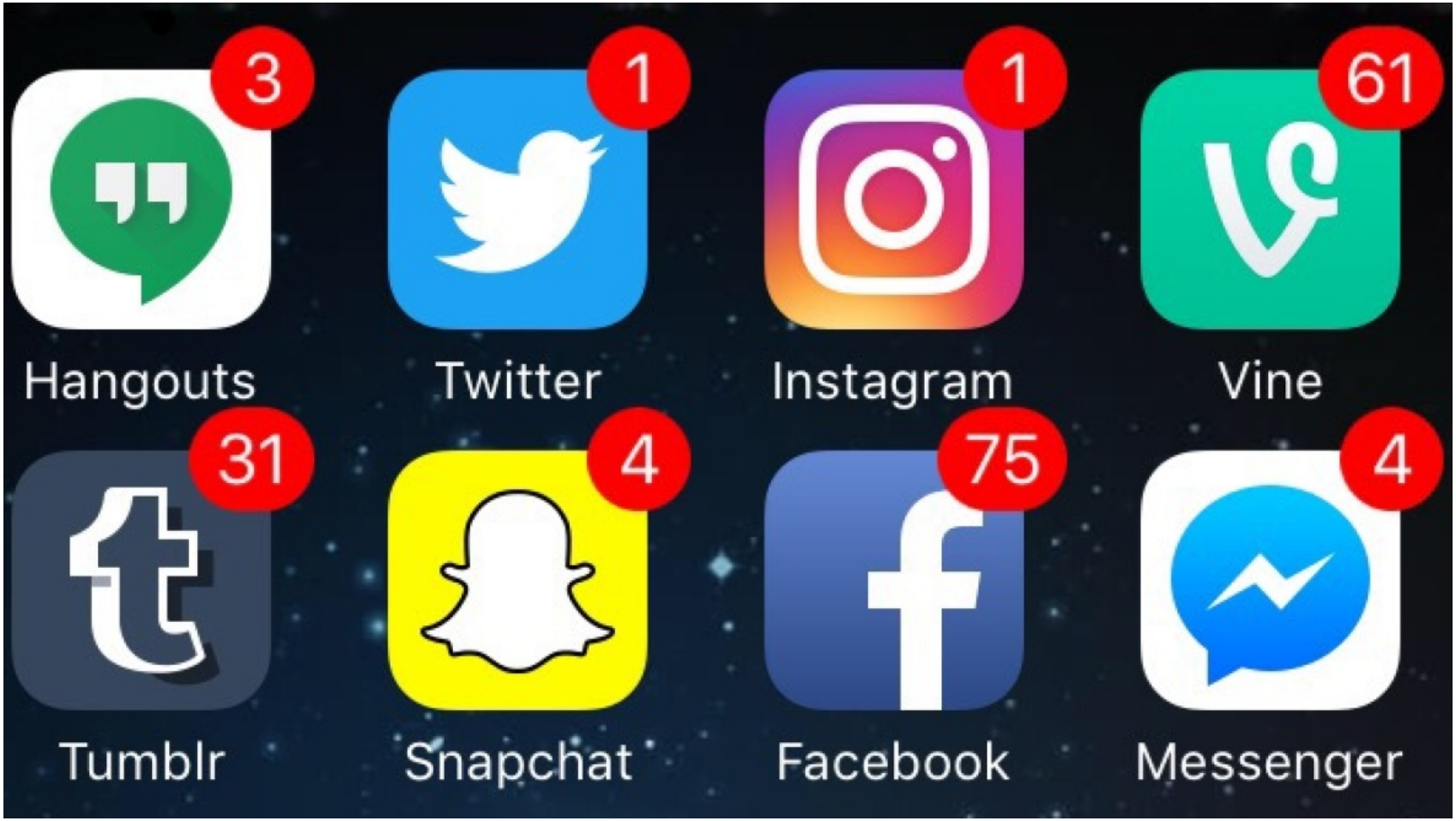
	amrita	**are**	**cen**	**cbe**	**in**	**is**	**we**
S1	0	1	1	0	1	0	1
S2	1	0	1	0	1	1	0
S3	1	0	0	1	1	1	0

Image to Matrix



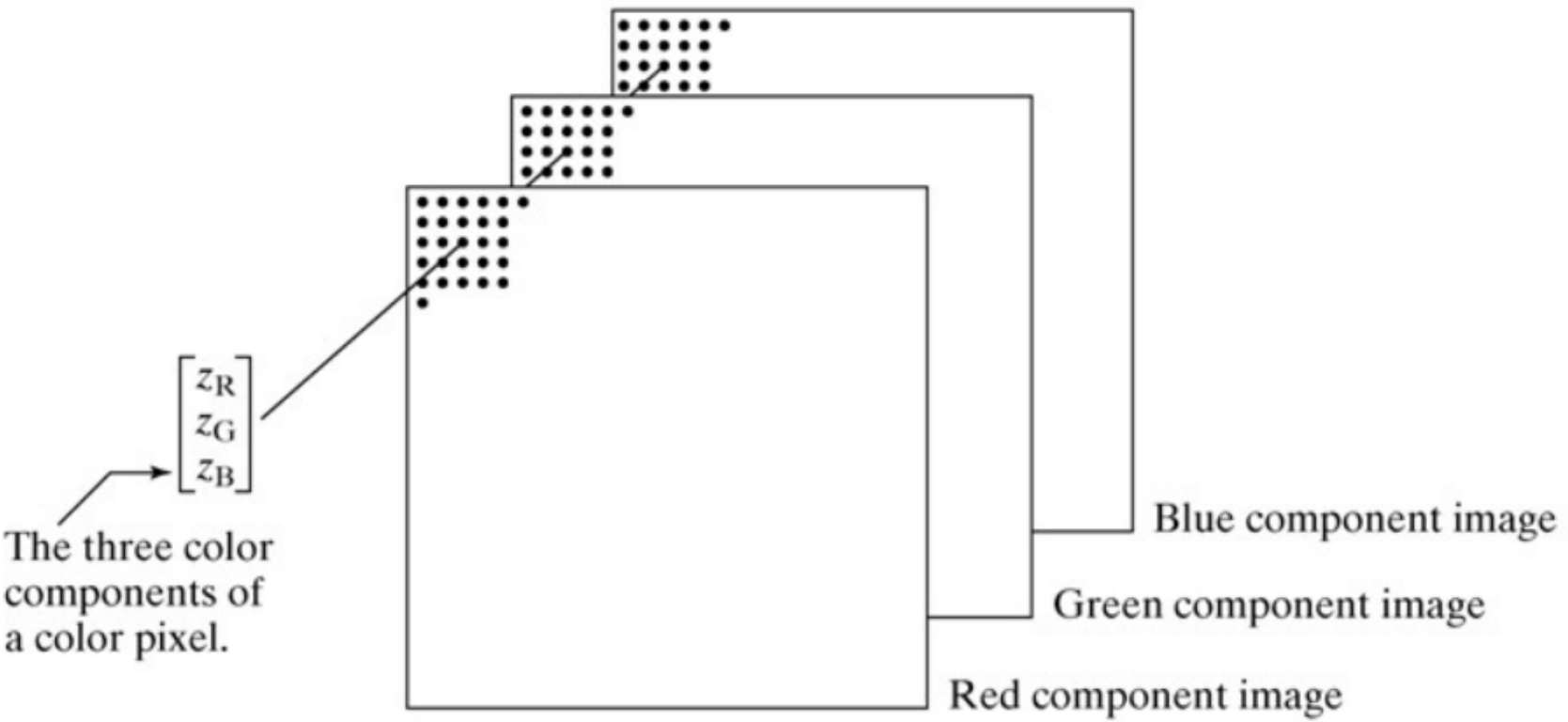
Source: http://blog.kleinproject.org/?p=588

Image to Matrix



Source: `http://www.cbc.ca/news/trending`

Image to Matrix



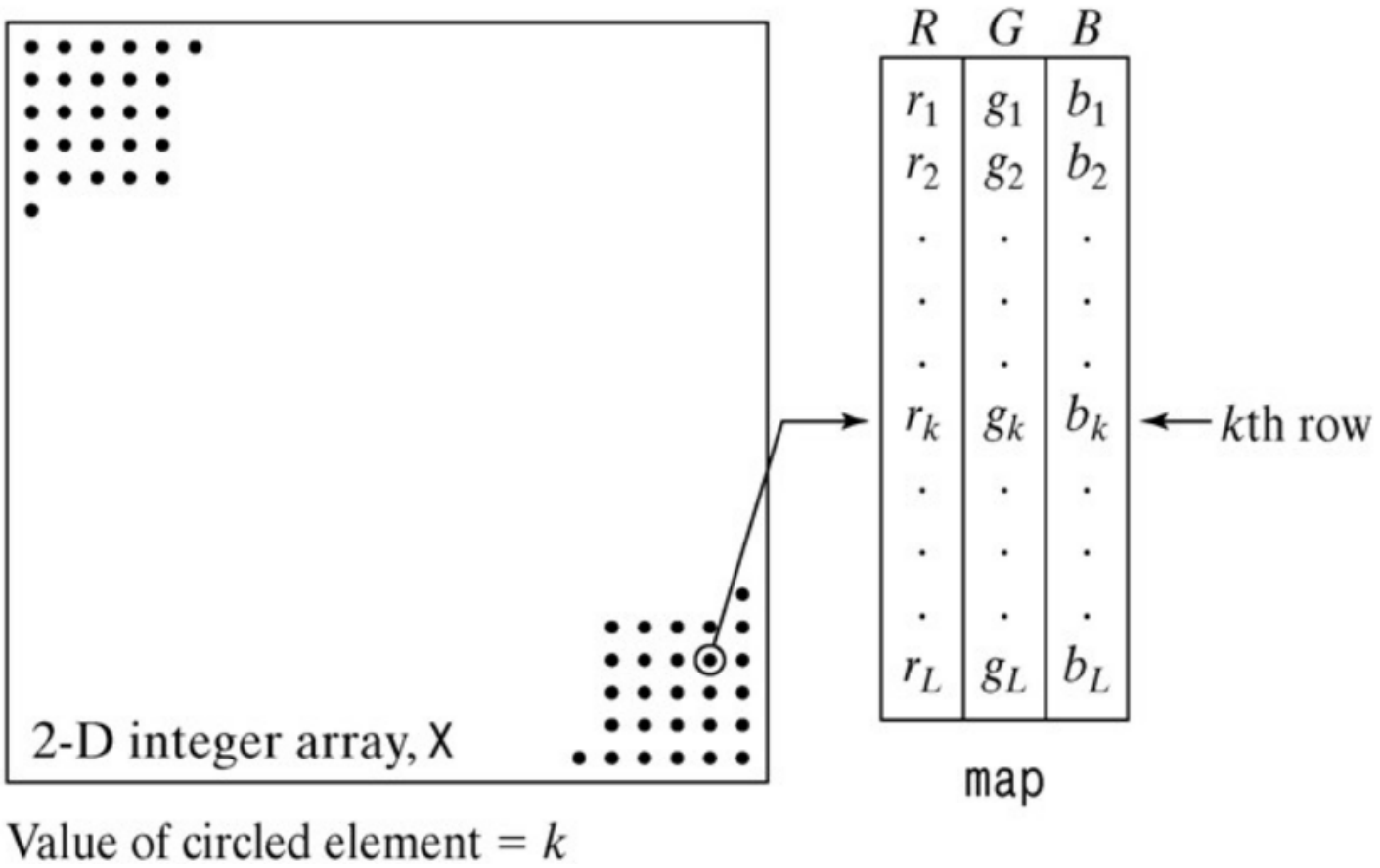
Source: `http://slideplayer.com/slide/8752313/`

Image to Matrix

88	82	84	88	85	83	80	93	102
88	80	78	80	80	78	73	94	100
85	79	80	78	77	74	65	91	99
38	35	40	35	39	74	77	70	65
20	25	23	28	37	69	64	60	57
22	26	22	28	40	65	64	59	34
24	28	24	30	37	60	58	56	66
21	22	23	27	38	60	67	65	67
23	22	22	25	38	59	64	67	66

Source: `http://www1.adept.com/main/KE/DATA/ACE/AdeptSight_User/Vision_Basics_Mode.html`

Image to Matrix



Source: http://slideplayer.com/slide/8752313/

From Regression to Deep Learning

$$2x = 6 \tag{6}$$

$$(2x - 6) = 0 \tag{7}$$

$$x = ? \tag{8}$$

$$2x = 6 \tag{9}$$

$$(2x - 6) = 0 \tag{10}$$

$$x = ? \tag{11}$$

$$x = 6/2 = 3 \tag{12}$$

$$2(3) - 6 = 0 \tag{13}$$

$$2a + b + c = 4 \tag{14}$$

$$a + 3b + 2c = 5 \tag{15}$$

$$a = 6 \tag{16}$$

$$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \tag{17}$$

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix}, x = \begin{bmatrix} a \\ b \\ c \end{bmatrix}, b = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \tag{18}$$

$$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \tag{19}$$

$$A\mathbf{x} = \mathbf{b} \tag{20}$$

$$(A\mathbf{x} - \mathbf{b}) = ? \tag{21}$$

$$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \tag{22}$$

$$A\mathbf{x} = \mathbf{b} \tag{23}$$

$$(A\mathbf{x} - \mathbf{b}) = 0 \tag{24}$$

$$\mathbf{x} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} = ? \tag{25}$$

What is Regression

$$x + y = z$$

What is Regression

$$2a + b + c = 4 \tag{26}$$

$$a + 3b + 2c = 5 \tag{27}$$

$$a = 6 \tag{28}$$

Solving Ax=b

$$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \tag{29}$$

$$A\ \mathbf{x} = \mathbf{b} \tag{30}$$

$$(A\ \mathbf{x} - \mathbf{b}) = 0 \tag{31}$$

$$\mathbf{x} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} = ? \tag{32}$$

$$A^{-1}\ A\ \mathbf{x} = A^{-1}\ \mathbf{b} \tag{33}$$

$$I\ \mathbf{x} = A^{-1}\ \mathbf{b} \tag{34}$$

$$\mathbf{x} = A^{-1}\ \mathbf{b} \tag{35}$$

House Rent Prediction

ID	AC	Area	#Bath	#Bed	Rent
1	0	1317	1	3	**30000**
2	0	1152	2	2	**27000**
3	0	816	1	2	**20000**
4	0	1111	1	3	**25000**
5	0	1605	2	3	**35000**
6	1	1077	1	2	**31000**
7	1	1040	1	3	**33000**
8	1	1114	1	3	**34000**
9	1	1795	2	3	**45000**
10	1	1296	2	2	**38000**

$$\begin{bmatrix} 0 & 1317 & 1 & 3 \\ 0 & 1152 & 2 & 2 \\ 0 & 816 & 1 & 2 \\ 0 & 1111 & 1 & 3 \\ 0 & 1605 & 2 & 3 \\ 1 & 1077 & 1 & 2 \\ 1 & 1040 & 1 & 3 \\ 1 & 1114 & 1 & 3 \\ 1 & 1795 & 2 & 3 \\ 1 & 1296 & 2 & 2 \end{bmatrix} \begin{bmatrix} w1 \\ w2 \\ w3 \\ w4 \end{bmatrix} = \begin{bmatrix} 30000 \\ 27000 \\ 20000 \\ 25000 \\ 35000 \\ 31000 \\ 33000 \\ 34000 \\ 45000 \\ 38000 \end{bmatrix} \tag{36}$$

$$X\ \mathbf{w} = \mathbf{y} \tag{37}$$

$$X^{-1}\ X\ \mathbf{w} = X^{-1}\ \mathbf{y} \tag{38}$$

$$\mathbf{w} = X^{-1}\ \mathbf{y} \tag{39}$$

$$\mathbf{w} = X^{-1}\,\mathbf{y} = X^{-1}\begin{bmatrix}30000\\27000\\20000\\25000\\35000\\31000\\33000\\34000\\45000\\38000\end{bmatrix} = \begin{bmatrix}8117.9\\12.6\\3441.9\\2835.9\end{bmatrix} = \begin{bmatrix}w1\\w2\\w3\\w4\end{bmatrix} \tag{40}$$

$$X\ \mathbf{w} = \mathbf{y} \tag{41}$$

$$\begin{bmatrix} 0 & 1317 & 1 & 3 \\ 0 & 1152 & 2 & 2 \\ 0 & 816 & 1 & 2 \\ 0 & 1111 & 1 & 3 \\ 0 & 1605 & 2 & 3 \\ 1 & 1077 & 1 & 2 \\ 1 & 1040 & 1 & 3 \\ 1 & 1114 & 1 & 3 \\ 1 & 1795 & 2 & 3 \\ 1 & 1296 & 2 & 2 \end{bmatrix} \begin{bmatrix} 8117.9 \\ 12.6 \\ 3441.9 \\ 2835.9 \end{bmatrix} = \begin{bmatrix} 28500.7 \\ 27033.1 \\ 19368.6 \\ 25911.8 \\ 35562.0 \\ 30766.6 \\ 33137.4 \\ 34067.4 \\ 46067.7 \\ 36960.7 \end{bmatrix} \tag{42}$$

$$X\ \mathbf{w} = \mathbf{y}^{pre} \tag{43}$$

$$training\ error = abs(\mathbf{y} - \mathbf{y}^{pre}) \tag{44}$$

$$training\ \ error = sum(abs(\mathbf{y} - \mathbf{y}^{pre})) \tag{45}$$

$$\mathbf{y} - \mathbf{y}^{pre} = \begin{bmatrix} 30000 \\ 27000 \\ 20000 \\ 25000 \\ 35000 \\ 31000 \\ 33000 \\ 34000 \\ 45000 \\ 38000 \end{bmatrix} - \begin{bmatrix} 28500.7 \\ 27033.1 \\ 19368.6 \\ 25911.8 \\ 35562.0 \\ 30766.6 \\ 33137.4 \\ 34067.4 \\ 46067.7 \\ 36960.7 \end{bmatrix} = \begin{bmatrix} 1499.2 \\ -33.1 \\ 631.3 \\ -911.8 \\ -562.0 \\ 233.3 \\ -137.4 \\ -67.4 \\ -1067.7 \\ 1039.2 \end{bmatrix} \tag{46}$$

$$abs(\mathbf{y} - \mathbf{y}^{pre}) = \begin{bmatrix} 1499.2 \\ 33.1 \\ 631.3 \\ 911.8 \\ 562.0 \\ 233.3 \\ 137.4 \\ 67.4 \\ 1067.7 \\ 1039.2 \end{bmatrix} \tag{47}$$

$$sum(abs(\mathbf{y} - \mathbf{y}^{pre})) = 6182.9 \tag{48}$$

$$\begin{bmatrix} AC & Area & Bath & Bed \end{bmatrix} \begin{bmatrix} 8117.9 \\ 12.6 \\ 3441.9 \\ 2835.9 \end{bmatrix} = [Price] \tag{49}$$

$$\mathbf{8117.9\ AC + 12.6\ Area + 3441.9\ Bath + 2835.9\ Bed = Price} \tag{50}$$

What is Classification

Classification?

House Price Prediction

ID	AC	Area	#Bath	#Bed	#Price	Decision
1	0	1317	1	3	**30000**	**1**
2	0	1152	2	2	**27000**	**0**
3	0	816	1	2	**20000**	**0**
4	0	1111	1	3	**25000**	**0**
5	0	1605	2	3	**35000**	**1**
6	1	1077	1	2	**31000**	**1**
7	1	1040	1	3	**33000**	**1**
8	1	1114	1	3	**34000**	**1**
9	1	1795	2	3	**45000**	**0**
10	1	1296	2	2	**38000**	**0**

$$\begin{bmatrix} AC & Area & Bath & Bed \end{bmatrix} \begin{bmatrix} 8117.9 \\ 12.6 \\ 3441.9 \\ 2835.9 \end{bmatrix} = [Price] \tag{51}$$

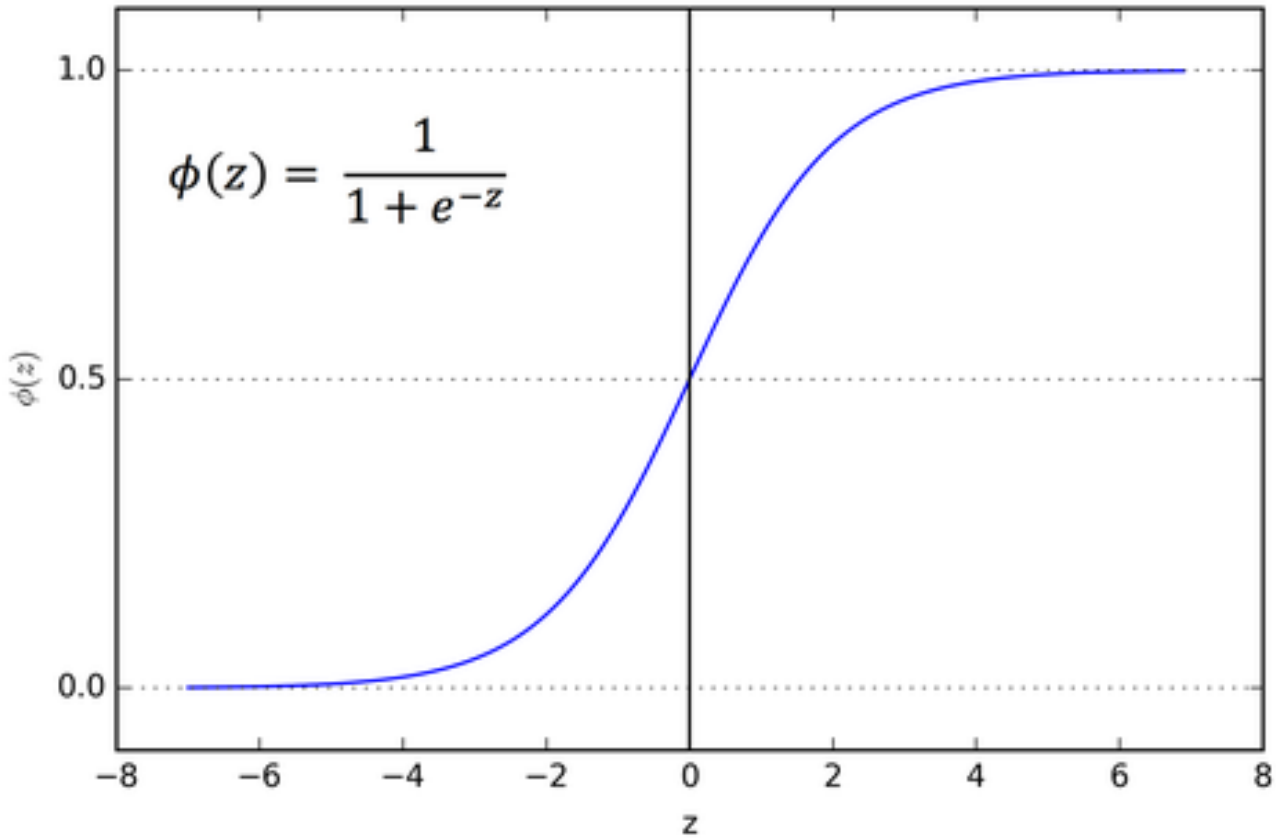
$$\mathbf{8117.9\ AC + 12.6\ Area + 3441.9\ Bath + 2835.9\ Bed = Price} \tag{52}$$

$$Prediction = \begin{cases} 1 & if\ 30000 \leqslant price \geqslant 35000 \\ 0 & else \end{cases} \tag{53}$$

Logistic Regression ?

Logistic + Regression

Logistic - Sigmoid



https://sebastianraschka.com/images/faq/logisticregr-neuralnet/sigmoid.png

Logistic - Sigmoid

$$\Phi(z) = \frac{1}{1 + exp^{-z}} \tag{54}$$

$$\Phi(-6) = \frac{1}{1 + exp^{-(-6)}} = \frac{1}{1 + 403.42} = 0.0024 \tag{55}$$

$$\Phi(0) = \frac{1}{1 + exp^{0}} = \frac{1}{1 + 1} = 0.5 \tag{56}$$

$$\Phi(6) = \frac{1}{1 + exp^{-(6)}} = \frac{1}{1 + 0.0024} = 0.997 \tag{57}$$

Logistic Regression

$$\Phi(z) = \frac{1}{1 + exp^{-z}} \tag{58}$$

$$\mathbf{y} = \Phi(X\ \mathbf{w}) = \frac{1}{1 + exp^{-(X\ \mathbf{w})}} \tag{59}$$

House Rent Prediction

ID	AC	Area	#Bath	#Bed	#Price	Decision
1	0	1317	1	3	**30000**	**1**
2	0	1152	2	2	**27000**	**0**
3	0	816	1	2	**20000**	**0**
4	0	1111	1	3	**25000**	**0**
5	0	1605	2	3	**35000**	**1**
6	1	1077	1	2	**31000**	**1**
7	1	1040	1	3	**33000**	**1**
8	1	1114	1	3	**34000**	**1**
9	1	1795	2	3	**45000**	**0**
10	1	1296	2	2	**38000**	**0**

$$\begin{bmatrix} AC & Area & Bath & Bed \end{bmatrix} \begin{bmatrix} 8117.9 \\ 12.6 \\ 3441.9 \\ 2835.9 \end{bmatrix} = [Price] \tag{60}$$

$$\mathbf{8117.9\ AC + 12.6\ Area + 3441.9\ Bath + 2835.9\ Bed = Price} \tag{61}$$

$$Prediction = \begin{cases} 1 & if\ 30000 \leqslant price \geqslant 35000 \\ 0 & else \end{cases} \tag{62}$$

$$\begin{bmatrix} 0 & 1317 & 1 & 3 \\ 0 & 1152 & 2 & 2 \\ 0 & 816 & 1 & 2 \\ 0 & 1111 & 1 & 3 \\ 0 & 1605 & 2 & 3 \\ 1 & 1077 & 1 & 2 \\ 1 & 1040 & 1 & 3 \\ 1 & 1114 & 1 & 3 \\ 1 & 1795 & 2 & 3 \\ 1 & 1296 & 2 & 2 \end{bmatrix} \begin{bmatrix} w1 \\ w2 \\ w3 \\ w4 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \tag{63}$$

$$X\ \mathbf{w} = \mathbf{y} \tag{64}$$

$$X^{-1}\ X\ \mathbf{w} = X^{-1}\ \mathbf{y} \tag{65}$$

$$\mathbf{w} = X^{-1}\ \mathbf{y} \tag{66}$$

$$\mathbf{w} = X^{-1}\,\mathbf{y} = X^{-1}\begin{bmatrix}1\\0\\0\\0\\1\\1\\1\\1\\0\\0\end{bmatrix} = \begin{bmatrix}0.171\\0.00052\\-0.568\\0.217\end{bmatrix} = \begin{bmatrix}w1\\w2\\w3\\w4\end{bmatrix} \tag{67}$$

$$\begin{bmatrix} 0 & 1317 & 1 & 3 \\ 0 & 1152 & 2 & 2 \\ 0 & 816 & 1 & 2 \\ 0 & 1111 & 1 & 3 \\ 0 & 1605 & 2 & 3 \\ 1 & 1077 & 1 & 2 \\ 1 & 1040 & 1 & 3 \\ 1 & 1114 & 1 & 3 \\ 1 & 1795 & 2 & 3 \\ 1 & 1296 & 2 & 2 \end{bmatrix} \begin{bmatrix} 0.171 \\ 0.00052 \\ -0.568 \\ 0.217 \end{bmatrix} = sigmoid \left(\begin{bmatrix} 0.77077253 \\ -0.10045096 \\ 0.29211902 \\ 0.66318764 \\ 0.35313423 \\ 0.59914666 \\ 0.79682603 \\ 0.83547303 \\ 0.62308164 \\ 0.14547264 \end{bmatrix} \right) \tag{68}$$

$$X\ \mathbf{w} = sigmoid(\mathbf{y}^{pre}) \tag{69}$$

$$sigmoid\left(\begin{bmatrix} 0.77077253 \\ -0.10045096 \\ 0.29211902 \\ 0.66318764 \\ 0.35313423 \\ 0.59914666 \\ 0.79682603 \\ 0.83547303 \\ 0.62308164 \\ 0.14547264 \end{bmatrix}\right) = \begin{bmatrix} 0.68368798 \\ 0.47490836 \\ 0.57251482 \\ 0.65997608 \\ 0.58737741 \\ 0.64546105 \\ 0.68929513 \\ 0.69751093 \\ 0.65091909 \\ 0.53630416 \end{bmatrix} \tag{70}$$

$$X\ \mathbf{w} = sigmoid(\mathbf{y}^{pre}) \tag{71}$$

$$training\ \ error = sum(abs(\mathbf{y} - sigmoid(\mathbf{y}^{pre}))) \tag{72}$$

$$training\ \ error = sum(abs(\mathbf{y} - sigmoid(\mathbf{y}^{pre})) \tag{73}$$

$$abs(\mathbf{y} - sigmoid(\mathbf{y}^{pre}) = \begin{bmatrix}1\\0\\0\\0\\1\\1\\1\\1\\0\\0\end{bmatrix} - \begin{bmatrix}0.68368798\\0.47490836\\0.57251482\\0.65997608\\0.58737741\\0.64546105\\0.68929513\\0.69751093\\0.65091909\\0.53630416\end{bmatrix} = \begin{bmatrix}0.31631202\\0.47490836\\0.57251482\\0.65997608\\0.41262259\\0.35453895\\0.31070487\\0.30248907\\0.65091909\\0.53630416\end{bmatrix} \tag{74}$$

$$training\ \ error = 4.59 \tag{75}$$

$$\begin{bmatrix} 0.31631202 \\ 0.47490836 \\ 0.57251482 \\ 0.65997608 \\ 0.41262259 \\ 0.35453895 \\ 0.31070487 \\ 0.30248907 \\ 0.65091909 \\ 0.53630416 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \tag{76}$$

$$Prediction = \begin{cases} 1 & if \ \ sigmoid(\mathbf{y}^{pre}) \geqslant 0.5 \\ 0 & else \end{cases} \tag{77}$$

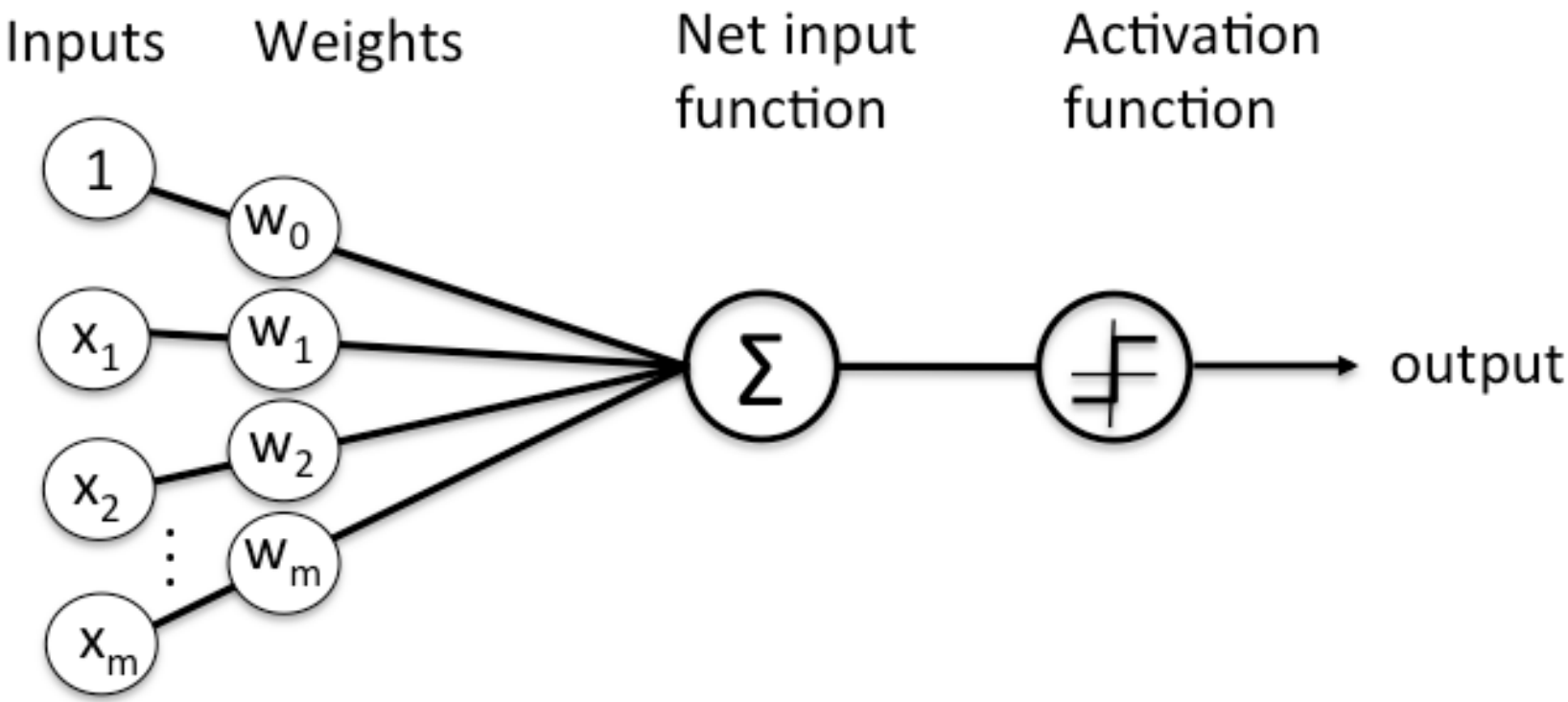
$$\begin{bmatrix} AC & Area & Bath & Bed \end{bmatrix} \begin{bmatrix} 0.171 \\ 0.00052 \\ -0.568 \\ 0.217 \end{bmatrix} = [Price] \tag{78}$$

$$\mathbf{0.171\ AC + 0.00052\ Area - 0.568\ Bath + 0.217\ Bed = Price} \tag{79}$$

$$sigmoid(\mathbf{y}^{pre}) = \frac{\mathbf{1}}{\mathbf{1 + exp^{-(0.171\ AC + 0.00052\ Area - 0.568\ Bath + 0.217\ Bed)}}} \tag{80}$$

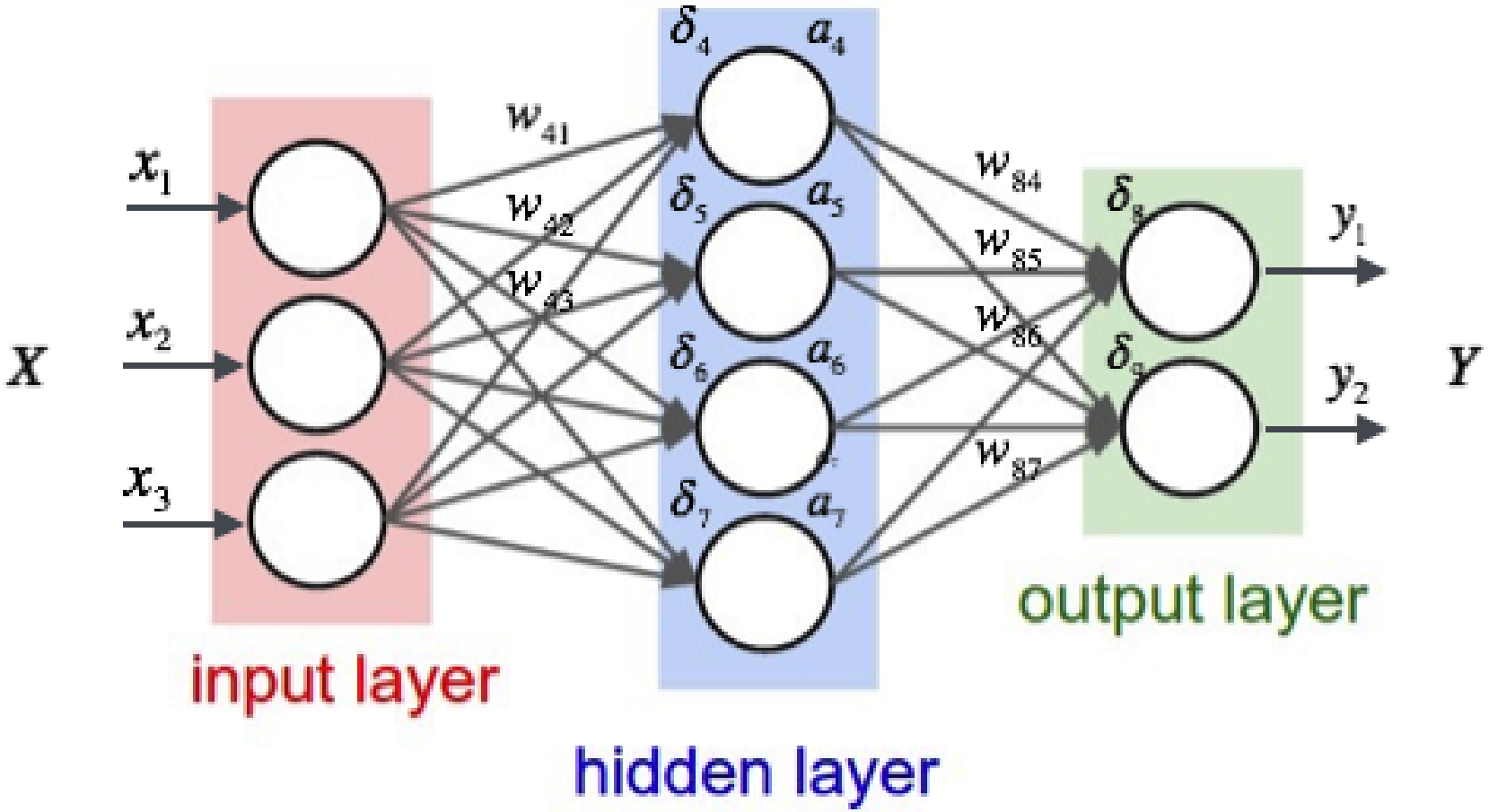
$$Prediction = \begin{cases} 1 & if\ \ sigmoid(\mathbf{y}^{pre}) \geqslant 0.5 \\ 0 & else \end{cases} \tag{81}$$

Logistic Regression as a Neuron



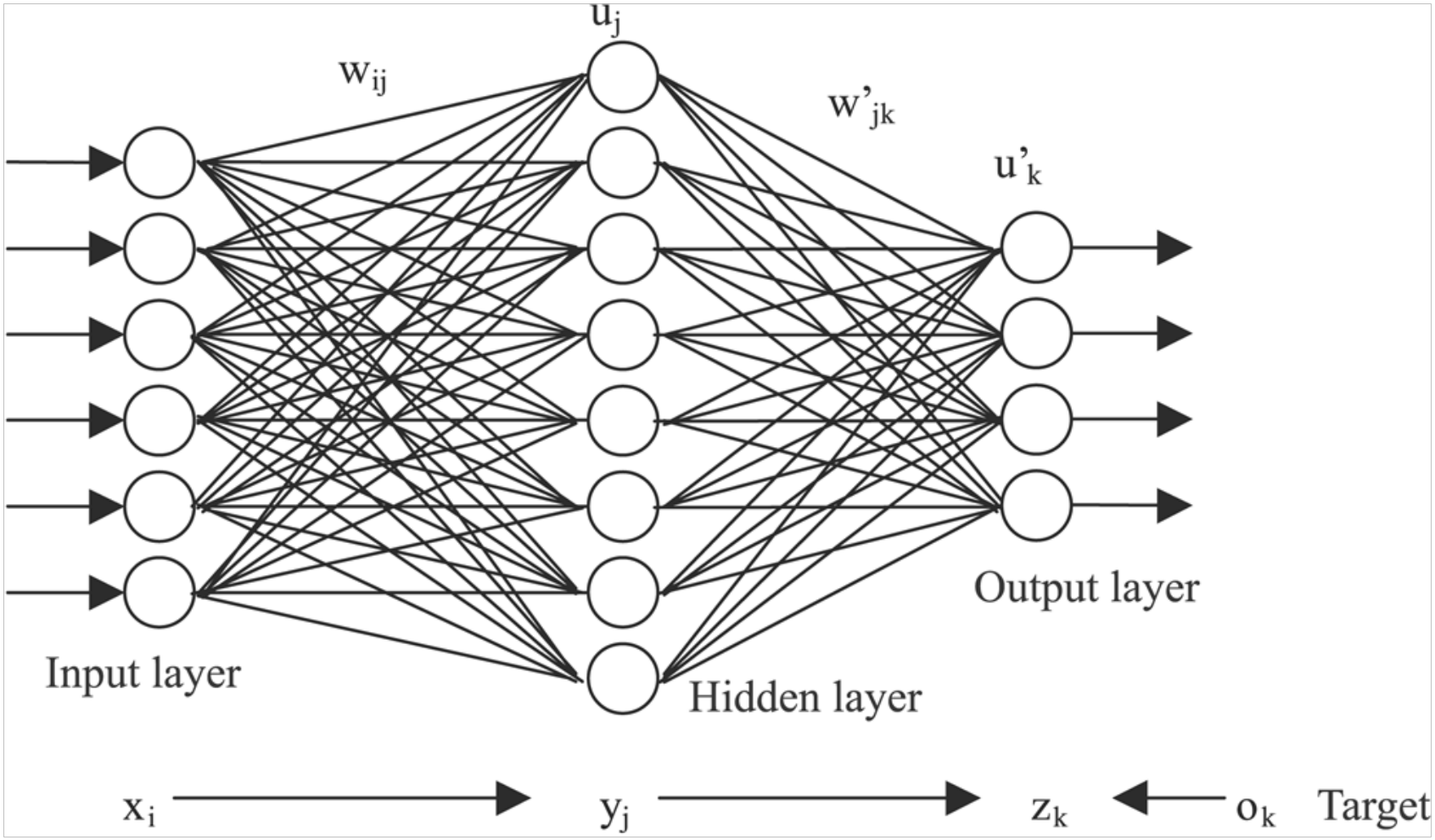
http://www.techmaru.com/technology/artificial-neural-networks/neural-network-elements

Neuron to Neurons



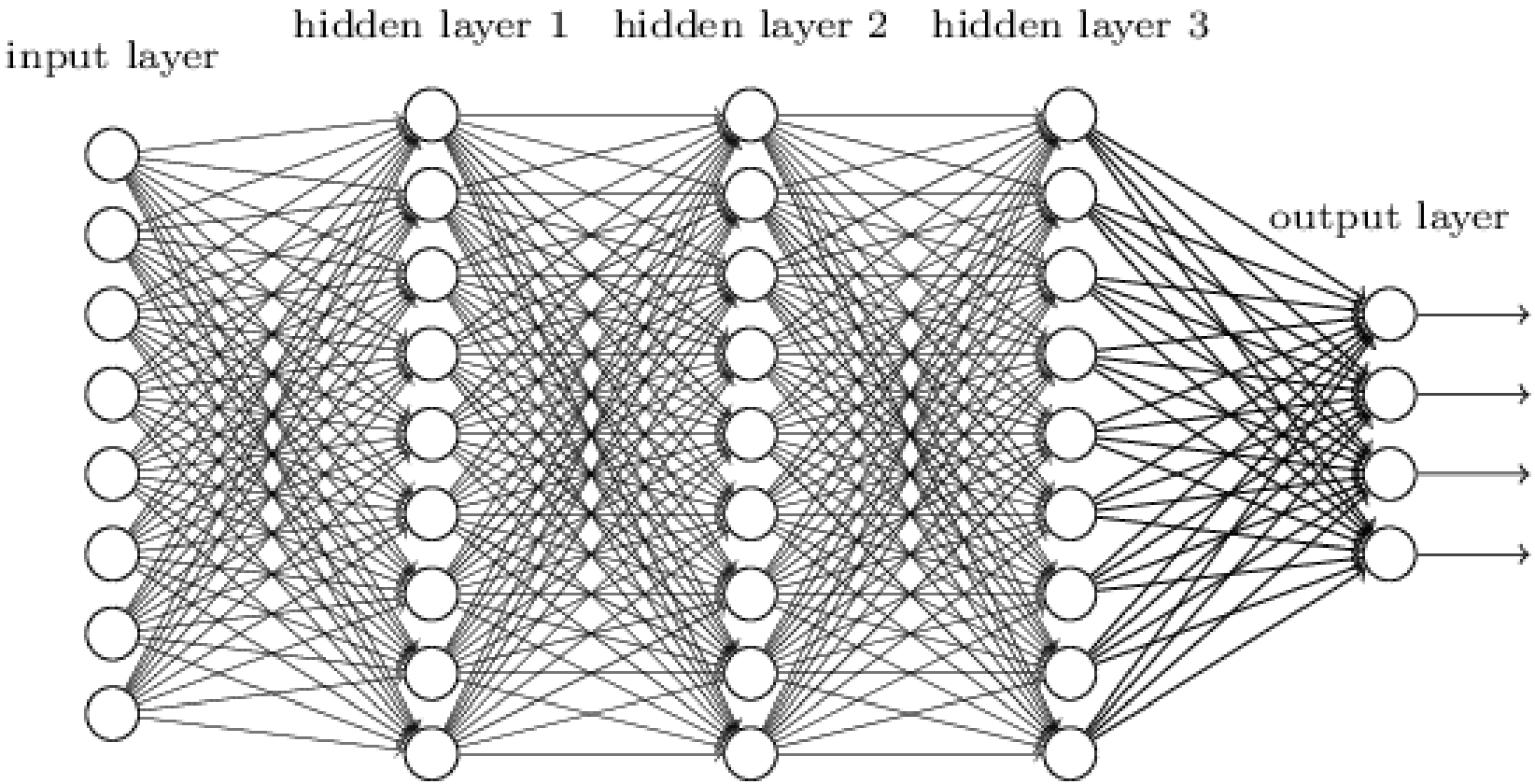
https://medium.com/@curiousily/tensorflow-for-hackers-part-iv-neural-network-from-scratch-1a4f504dfa8

Single Layer Network



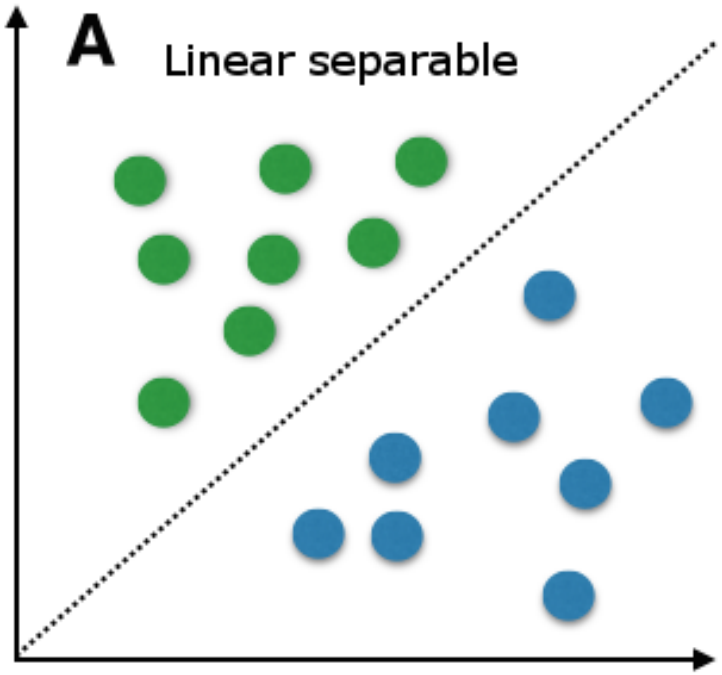
https://www.extremetech.com/extreme/215170-artificial-neural-networks-are-changing-the-world-what-are-they

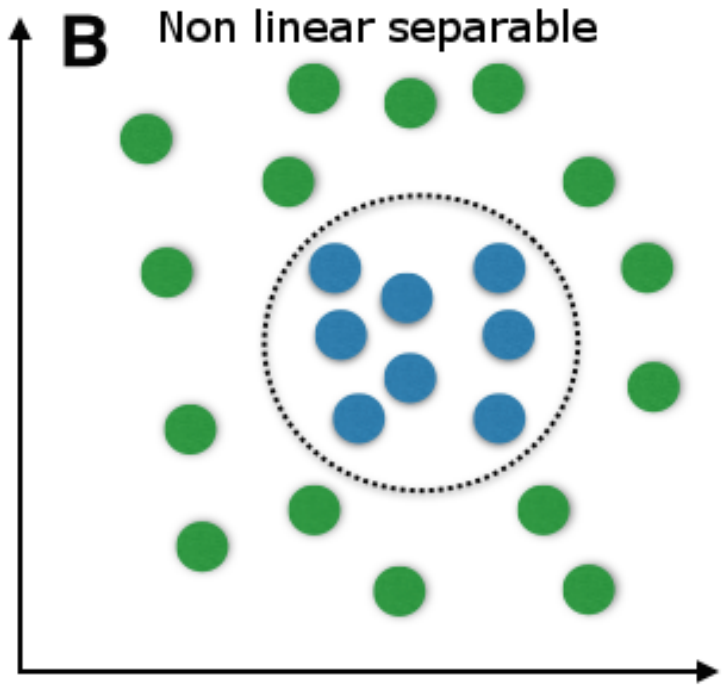
Multi Layer Network



https://in.mathworks.com/matlabcentral/fileexchange/64247-simple-neural-network

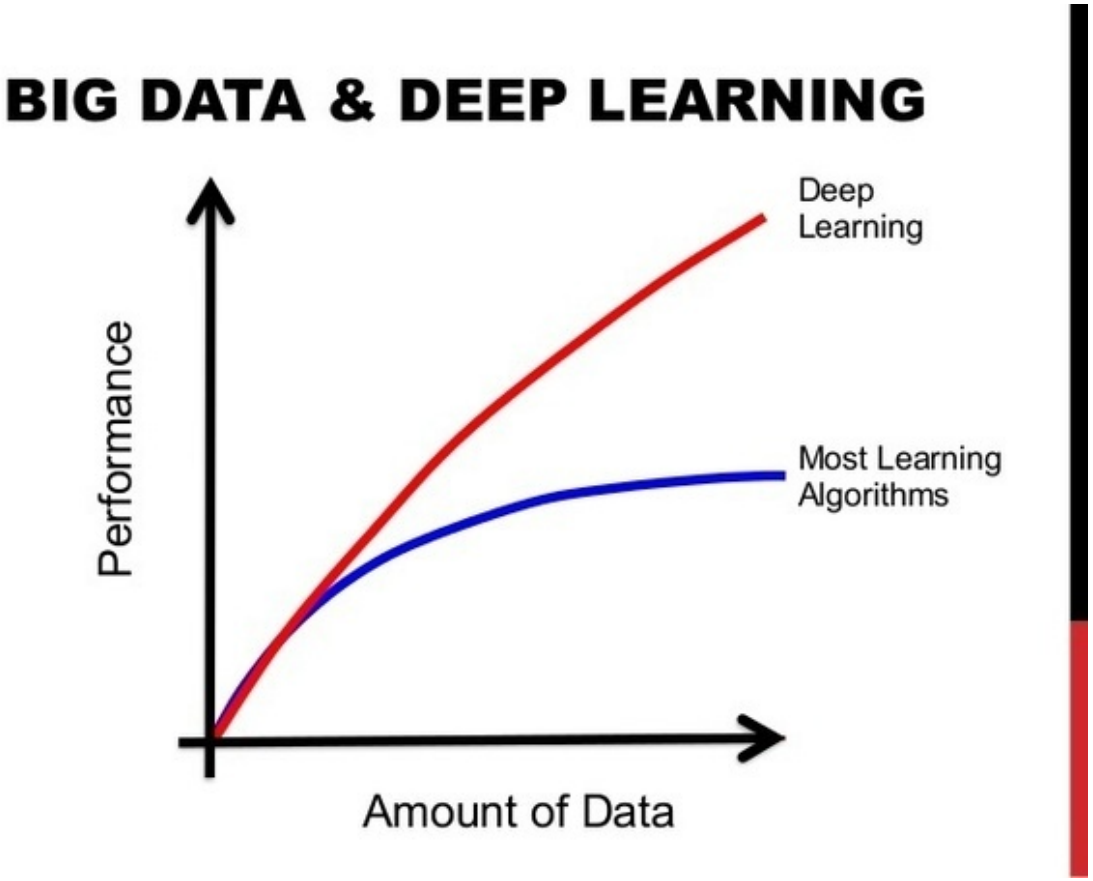
Why Deep Learning?





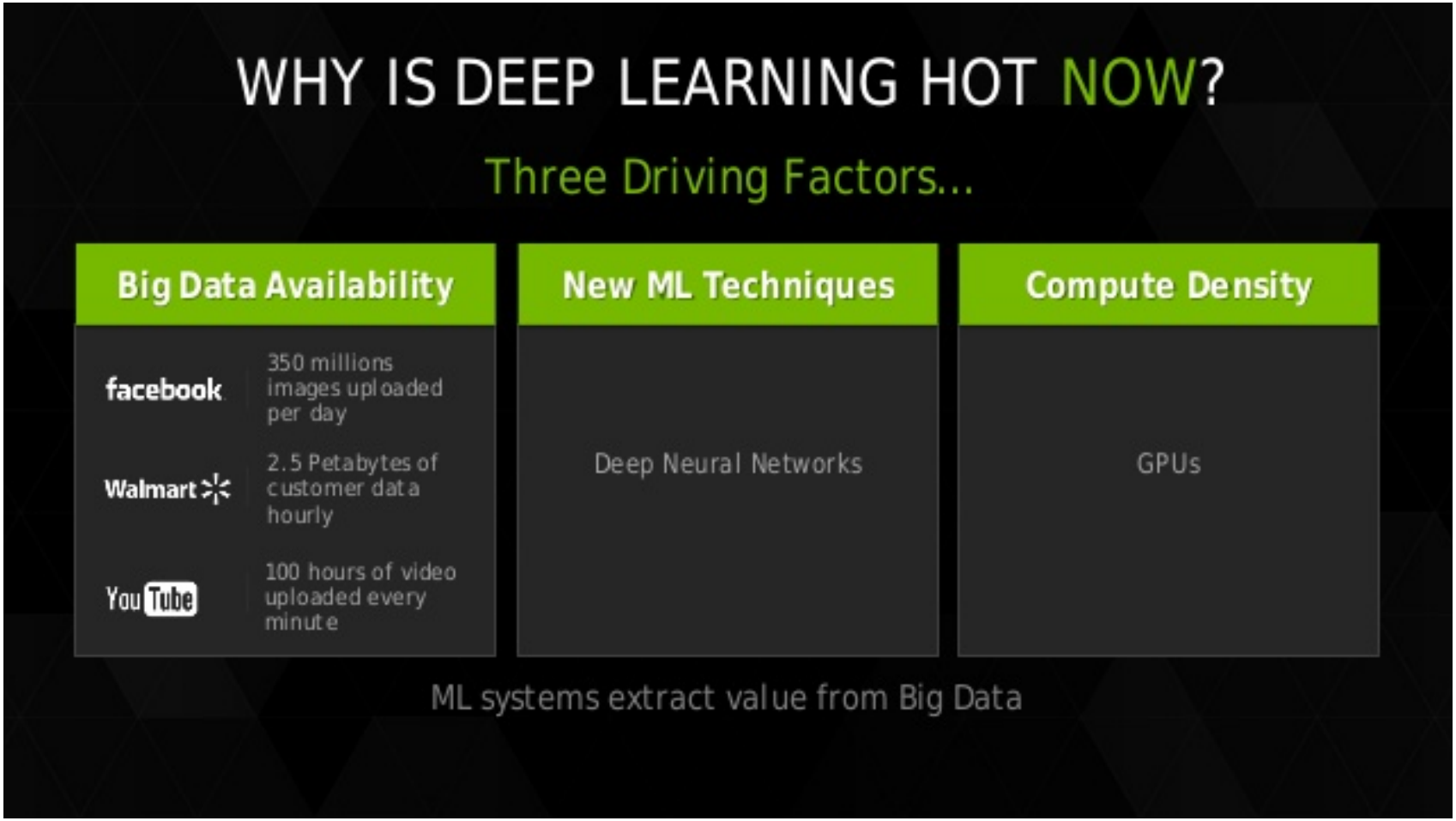
Source: https://leonardoaraujosantos.gitbooks.io/artificial-inteligence/content/linear_classification.html

Why Deep Learning?



Source: `https://qph.ec.quoracdn.net/main-qimg-bf69c291005e68620a1bef39ae8f029e-c`

Why now Deep Learning?



https://www.slideshare.net/DataScienceMD/deep-learning-with-gpus

Common Deep Learning Algorithms

- Convolutional Neural Network
- Recurrent Neural Network
- Long-Short Term Memory Network
- Deep Neural Network
- Auto Encoders

How to do Machine Learning?

- Collecting data
- Preparing the data
- Training a model
- Evaluating the model
- Improving the performance

Thank You.

you can follow me through:

www.linkedin.com/in/barathiganeshhb