COGS 118A, Winter 2020

Supervised Machine Learning Algorithms

Lecture 1: Basics

Zhuowen Tu

Vector

(probably the most important concept in this class)

Vector: a sequence of elements

(white, red, blue, green)

Important to note: the order DOES matter for vectors

(white, red, blue, green) $\neq$ (red, white, green, blue)

Sometimes, we also use: <white, red, blue, green>

In Python: [white, red, blue, green]

It is of critical importance to under the vector representation in machine learning!

Some notations that we will be using

Input data:

We use x (lower case) to denote a feature value (scalar).

The ith input data sample is represented as a vector using bold $\mathbf{x}$:

$\mathbf{x}_i = (x_{i1}, ..., x_{im}) \in \mathbb{R}^m$: A row vector of m elements.

$\mathbf{x}_i = (22, 1, 0, 160, 180)$

The entire dataset is represented by a set (the sequence in which each data input $\mathbf{x}_i$ usually doesn't matter.

$S = \{\mathbf{x}_i, i = 1..n\}$: A set S with n samples. i goes from 1 to n.

Some notations that we will be using

Output prediction:

We use y (lower case) to denote a binary classification.

$y = -1$ (or sometimes we use $y = 0$) is referred to as the negative class.

$y = +1$ is referred to as the positive class.

Given a data sample $\mathbf{x}_i = (x_{i1}, ..., x_{im})$,

we want to predict $y_i \stackrel{?}{=} -1 \; or \; +1$

Some notations that we will be using

Model parameter:

Model: $\mathbf{w} = (w_1, ..., w_m) \in \mathbb{R}^m$ (in the same dimension of input $\mathbf{x}$)

bias: $b \in \mathbb{R}$ (scalar)

Data sample $\mathbf{x} = (x_1, ..., x_m) \in \mathbb{R}^m$,

$\mathbf{w} \cdot \mathbf{x} + b$ $\qquad$ $y = \begin{cases} +1 & if \ \ \mathbf{w} \cdot \mathbf{x} + b \geq 0 \\ -1 & otherwise \end{cases}$ $\qquad$ $(w_1, w_2, .., w_m) \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ x_m \end{pmatrix} + b$

"$\cdot$" refers to as the dot product between two vectors

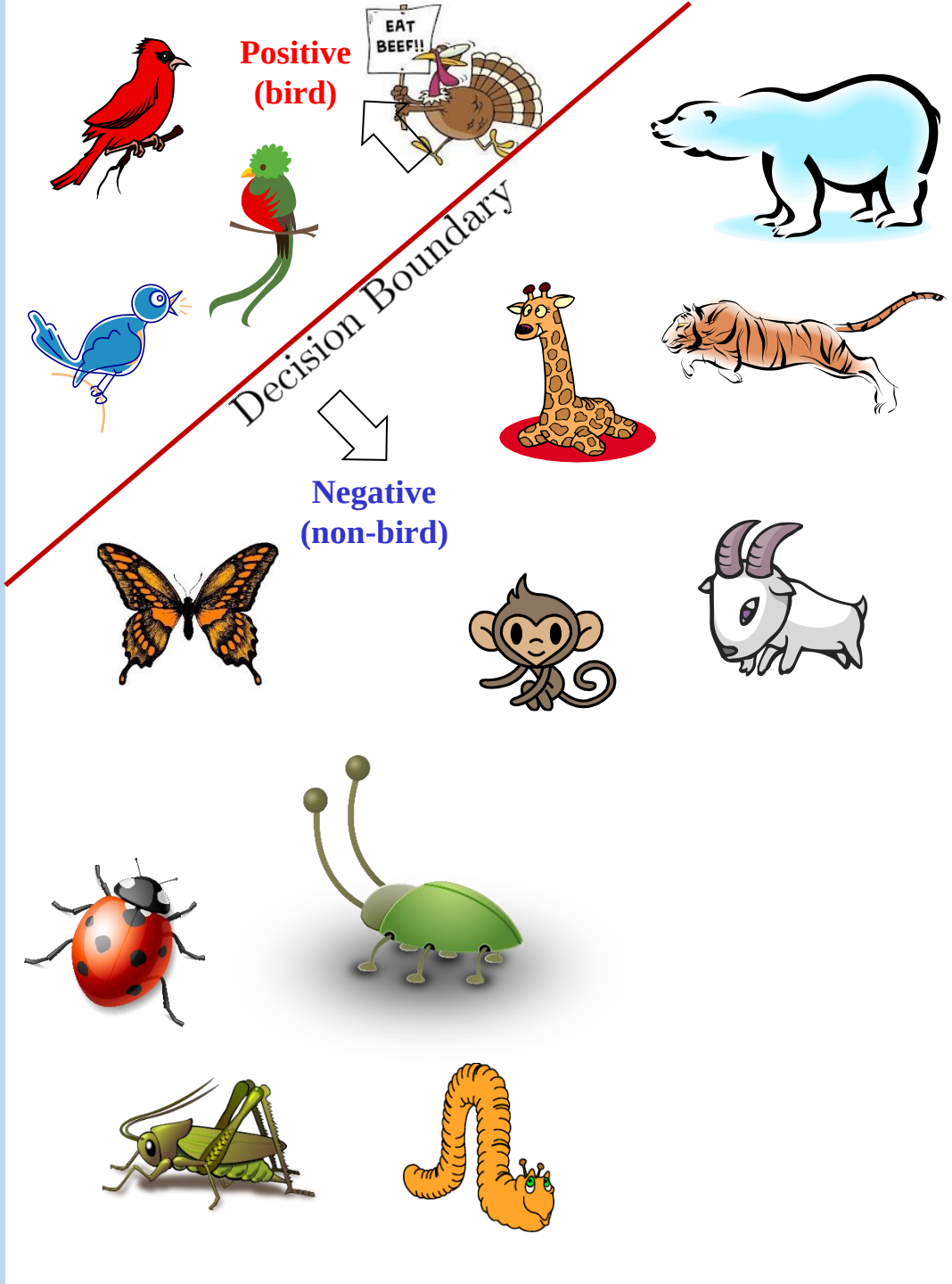
Alternative notation 1: $< \mathbf{w}, \mathbf{x} > + b$

Alternative notation 2: $\mathbf{w}\mathbf{x}^T + b$ ($\mathbf{w}$ and $\mathbf{x}$ are row vectors).

$\mathbf{w}^T\mathbf{x} + b$ ($\mathbf{w}$ and $\mathbf{x}$ are column vectors).

Supervised learning

(Classification)



Summary of the classification problem

$\mathbf{x} = (x_1, x_2, ...)$

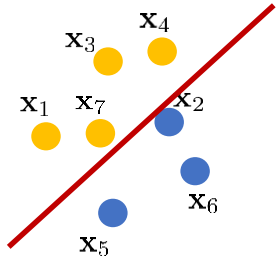
$y = 1(bird)$

x_1: color
x_2 weight
...

$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_3, y_3), (\mathbf{x}_4, y_4), (\mathbf{x}_5, y_5)\}$

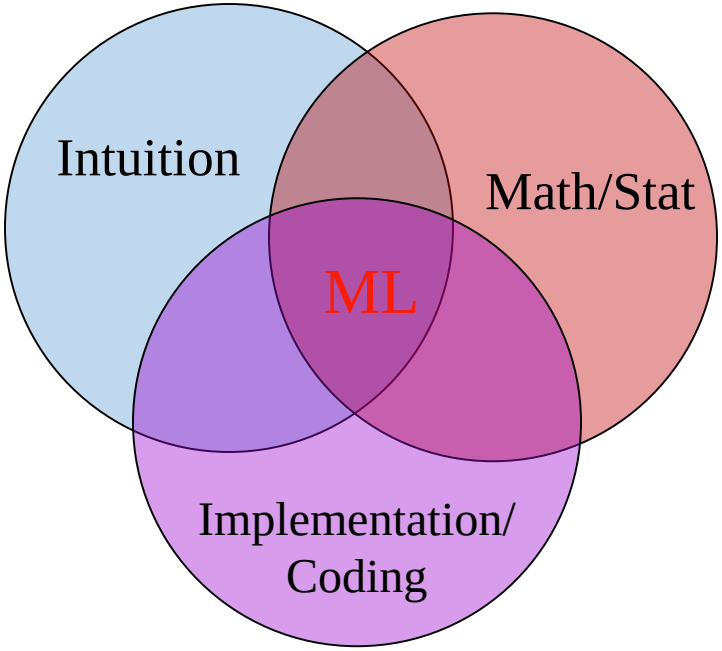
classifier $\mathbf{w} \cdot \mathbf{x} + b$

$\mathbf{w}, b$: model parameters



$\mathbf{w} \cdot \mathbf{x} + b$

A Big Picture



To do well in machine learning:

Intuition + Math/Stat +
Implementation/Coding

Basic concepts (supervised)

$$\mathbf{x}_i = (x_{i1}, ..., x_{im}), x_{ij} \in \mathbb{R}, \quad \mathbf{x} \in \mathbb{R}^m$$

$$y_i \in \mathbb{R}$$

Training (supervised)

$$S_{training} = \{(\mathbf{x}_i, y_i), i = 1..n\}$$

blood presure	age	male or female	weight (lb)	height (cm)
y_1=131	$x_{11} = 22$	$x_{12} = M$	$x_{13} = 160$	$x_{14} = 180$
y_2=150	$x_{21} = 51$	$x_{22} = M$	$x_{23} = 190$	$x_{24} = 175$
y_3=105	$x_{31} = 43$	$x_{32} = F$	$x_{33} = 120$	$x_{34} = 165$

In supervised setting during training, y_i (the solution) to each sample x_i is provided.

Supervised learning (training)

1. We are provided with a list of data samples in training.

2. In addition, each sample is associated with a label (-1 or +1 in binary classification), which is often manually (automatically, sometimes) delineated.

3. Our job is to use the provided training data to train to obtain a machine learning model for the future prediction.

4. In modern machine learning, the training process is often guided with principled mathematical formulations and algorithms.

Basic concepts (supervised)

$$\mathbf{x}_i = (x_{i1}, ..., x_{im}), x_{ij} \in \mathbb{R}, \quad \mathbf{x} \in \mathbb{R}^m$$

$$y_i \in \mathbb{R}$$

Testing:

$$S_{testing} = \{(\mathbf{x}_i), i = 1..u\}, what\ is\ y_i?$$

blood presure	age	male or female	weight (lb)	height (cm)
y_1=?	$x_{11} = 32$	$x_{12} = F$	$x_{13} = 130$	$x_{14} = 180$
y_2=?	$x_{21} = 11$	$x_{22} = M$	$x_{23} = 52$	$x_{24} = 135$

Supervised learning (testing)

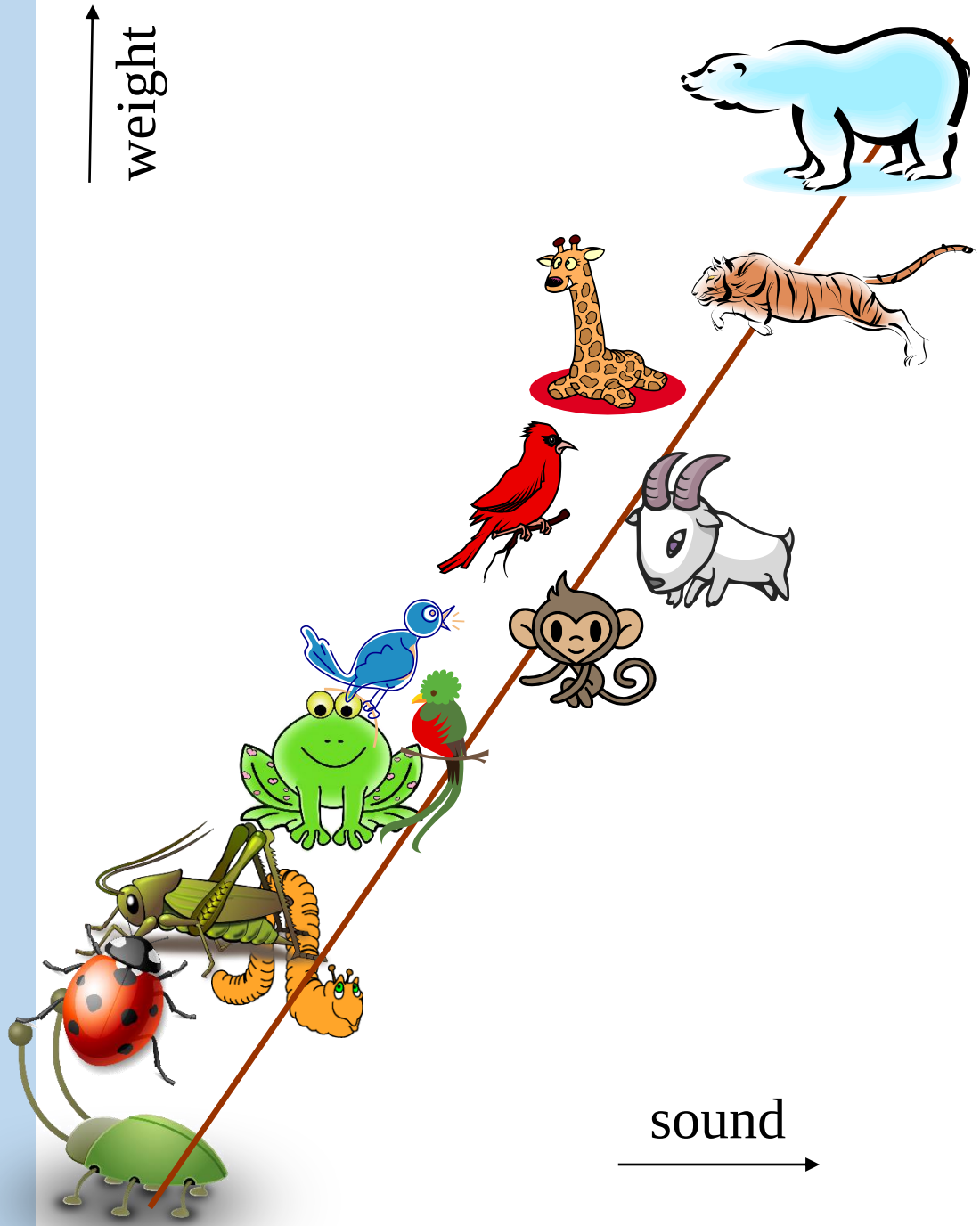
1. Given a model learned in the training process, we can make prediction in the “future” situations.

2. To be able to simulate and evaluate the performance of the learned model, we establish a “testing” dataset whose “ground-truth” labels are unknown for the model.

3. However, we still provide the “ground-truth” labels for the evaluation purposes.

Supervised learning

(Regression: weight prediction)



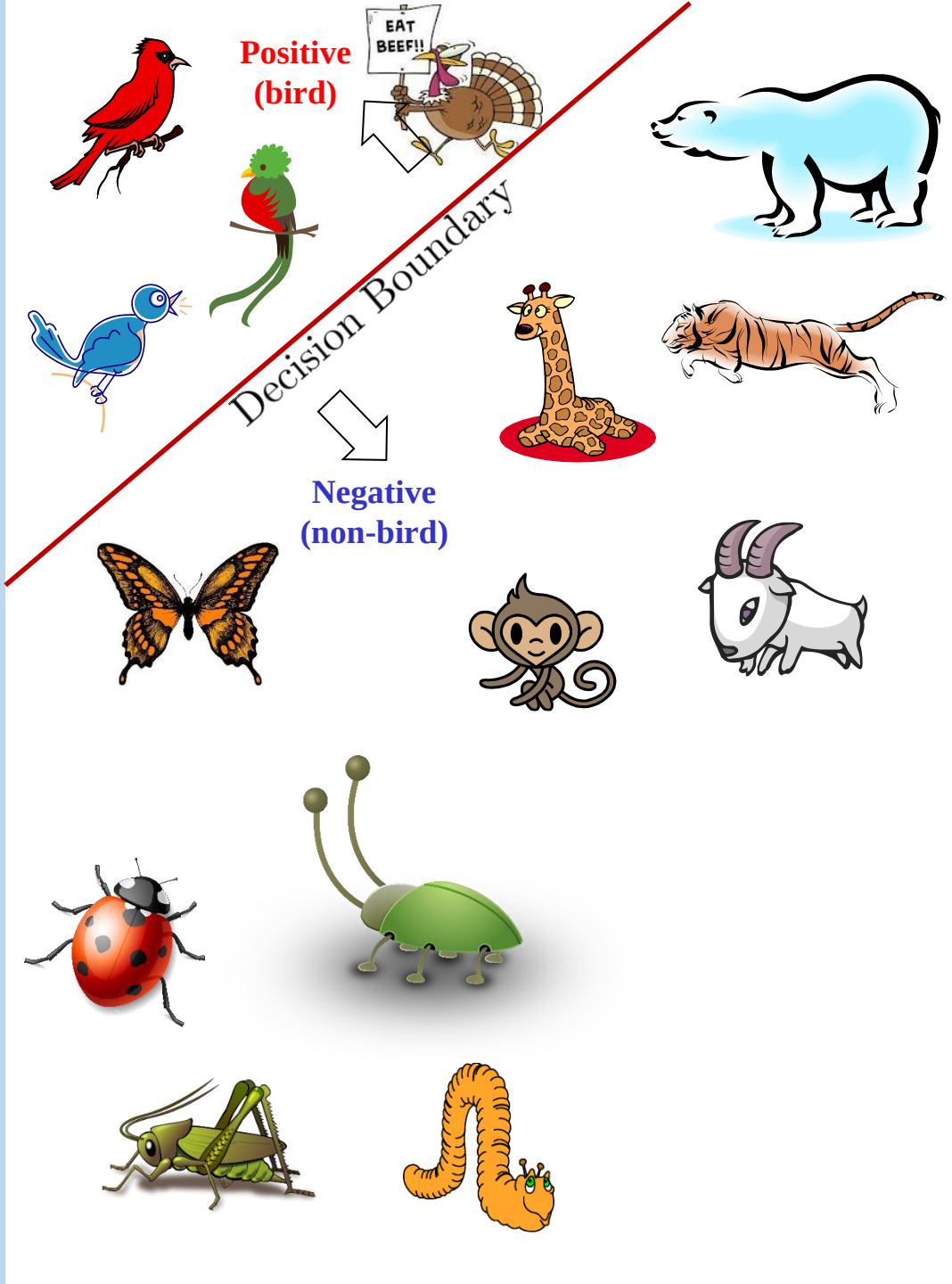
Regression

In regression, the “ground-truth” labels are continues values that are directly comparable.

That is, you can compare $y_1 = -1$ and $y_2 = 1$ to state for example $y_1 < y_2$ $(-1 < 1)$.

Supervised learning

(Classification)



Classification

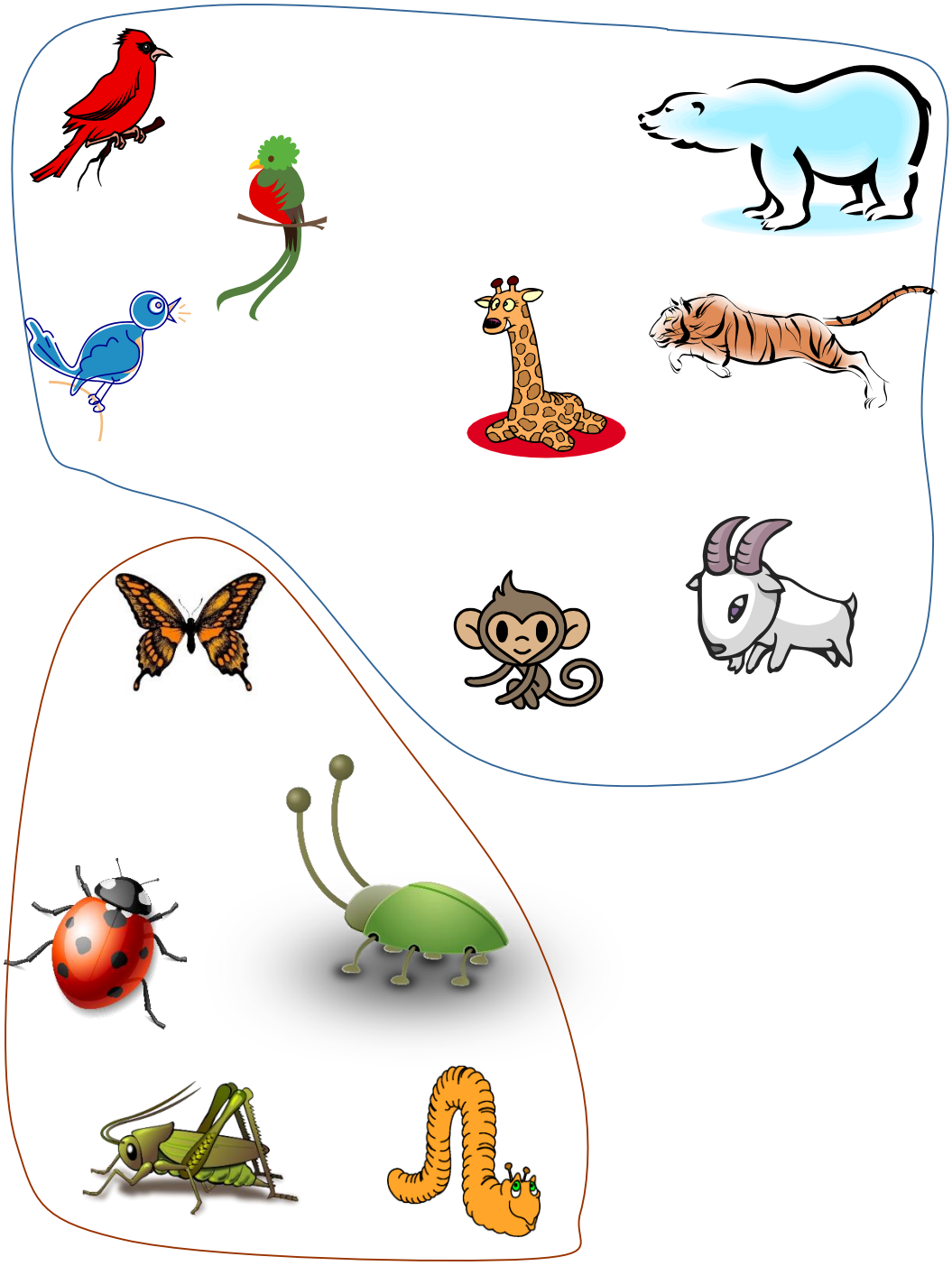
In classification, the "ground-truth" labels are categorical labels that are NOT directly comparable.

That is, you can not compare $y_1 =$ "$bird''$ and $y_2 =$ "$non - bird''$) to state for example:

"bird" $<$ "non-bird" (even we use $+1$ and -1 to denote their labels respectively).

Unsupervised learning

(Clustering)



Clustering (unsupervised)

In clustering, no “ground-truth” labels are given and our task is the separate the given samples into a number of ``groups”.

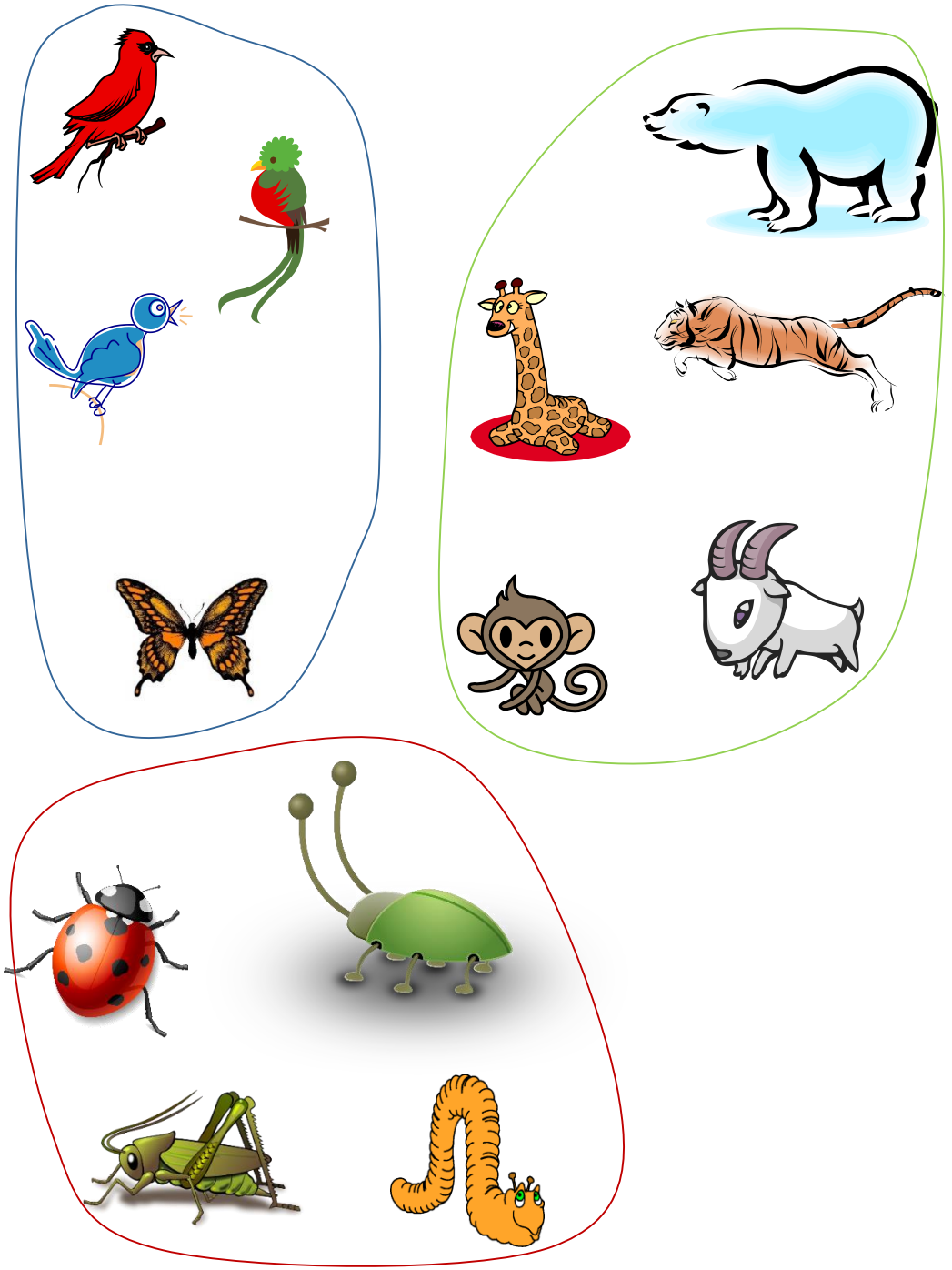
You need to decide:

1. How many groups are there.
2. How to group/divide them.

The clustering problem is unsupervised and consists of greater level of uncertainty, when compared with the supervised learning scenario.

Unsupervised learning

(Clustering results are not UNIQUE)



Features

What defines features?

How are they given?

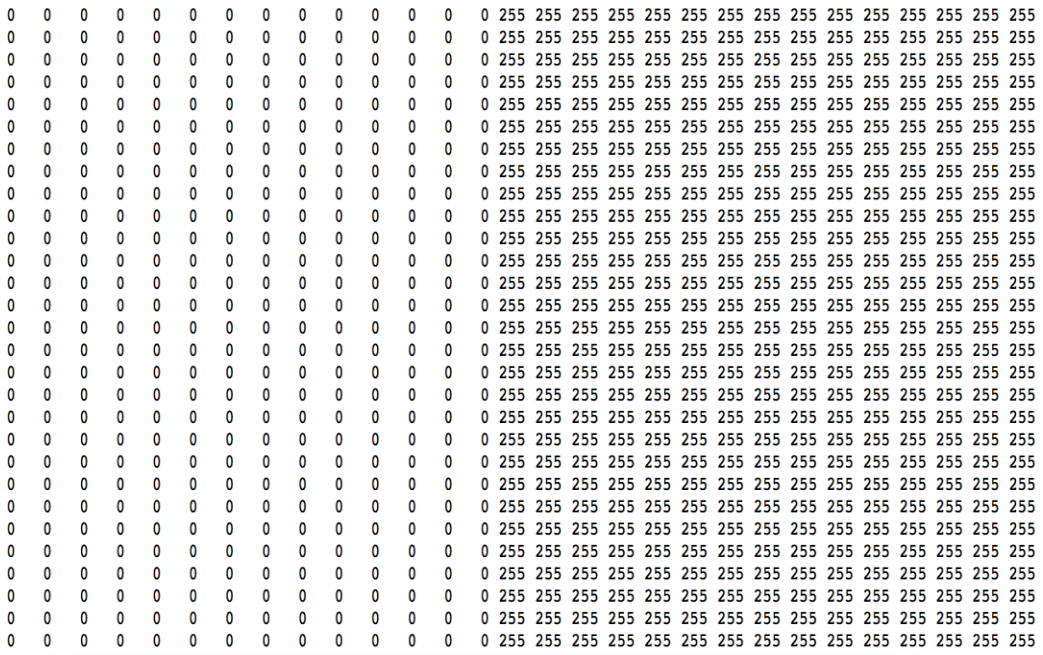
What is the difference between features and the input?

How to compute them?

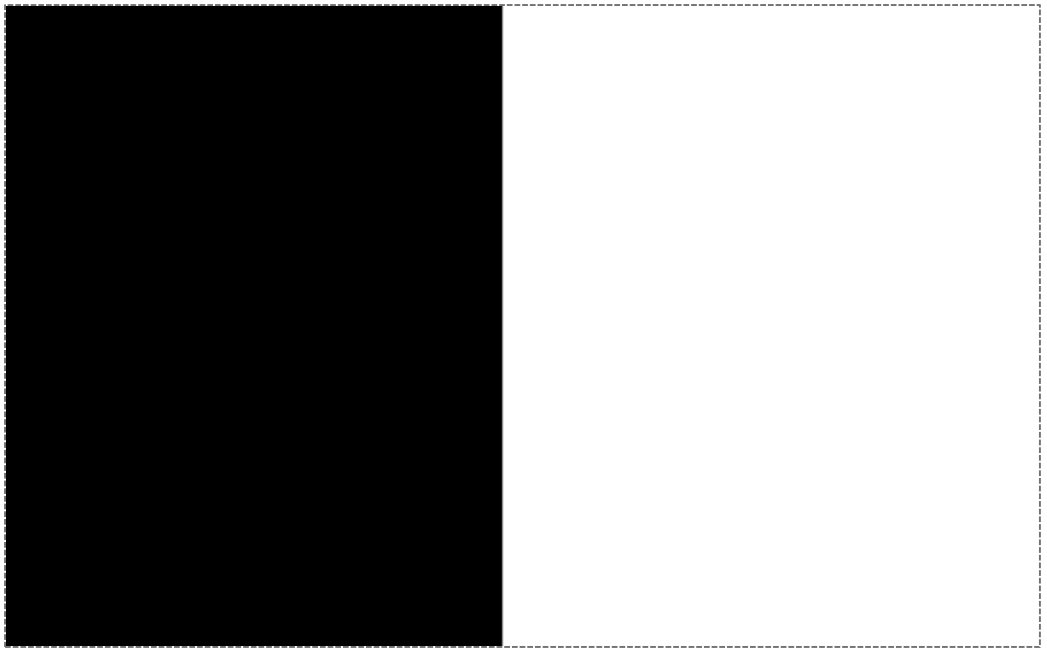
How to evaluate them?

How to use them?

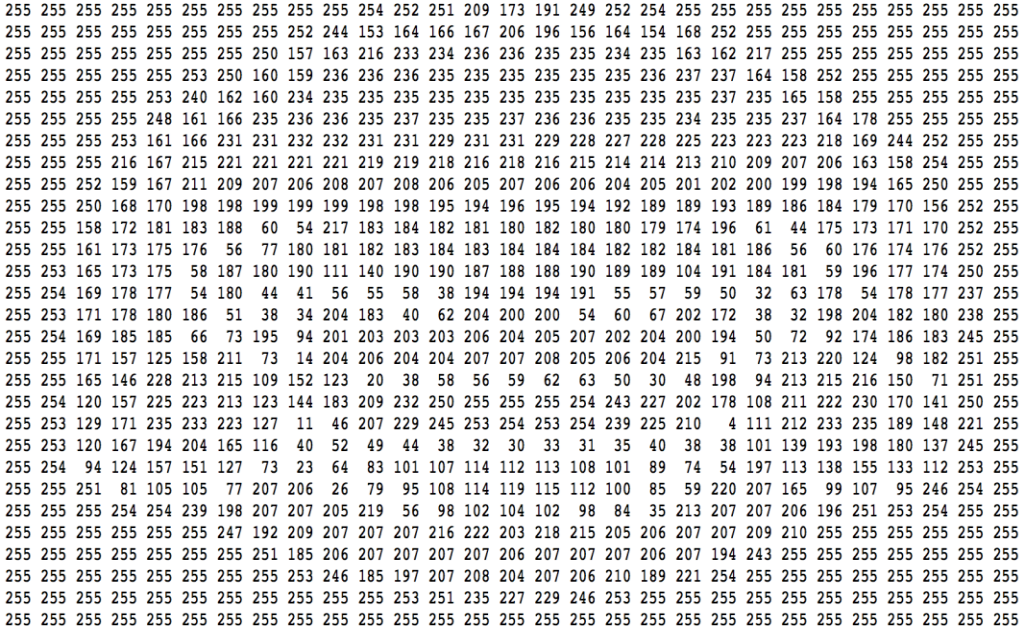
Why are features important



Why are features important



What is it?



A. Dog?

B. Chicken?

C. Car?

D. Elephant?

What is it?

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How to represent a raw image?

Each image is turned into a vector of size: $n \times m$

m: width

n : height

255	255	255	255	255	255	255	255	255	255	254	252	251	209	
255	255	255	255	255	255	255	255	255	252	244	153	164	166	167
255	255	255	255	255	255	255	250	157	163	216	233	234	236	
255	255	255	255	255	253	250	160	159	236	236	236	235	235	
255	255	255	255	253	240	162	160	234	235	235	235	235	235	
255	255	255	255	248	161	166	235	236	236	235	237	235	235	
255	255	255	253	161	166	231	231	232	232	231	231	229	231	
255	255	255	216	167	215	221	221	221	221	219	219	218	216	
255	255	252	159	167	211	209	207	206	208	207	208	206	205	
255	255	250	168	170	198	198	199	199	199	198	198	195	194	
255	255	158	172	181	183	188	60	54	217	183	184	182	181	
255	255	161	173	175	176	56	77	180	181	182	183	184	183	
255	253	165	173	175	58	187	180	190	111	140	190	190	187	
255	254	169	178	177	54	180	44	41	56	55	58	38	194	
255	253	171	178	180	186	51	38	34	204	183	40	62	204	
255	254	169	185	185	66	73	195	94	201	203	203	203	206	
255	255	171	157	125	158	211	73	14	204	206	204	204	207	
255	255	165	146	228	213	215	109	152	123	20	38	58	56	

Image Matrix

Image Vector

How to represent a raw image?

Each image is turned into a vector of size: $n \times m$

m: width

n : height

255	255	255	255	255	255	255	255	255	255	254	252	251	209
255	255	255	255	255	255	255	255	255	252	244	153	164	166	167
255	255	255	255	255	255	255	255	250	157	163	216	233	234	236
255	255	255	255	255	255	253	250	160	159	236	236	236	235	235
255	255	255	255	255	253	240	162	160	234	235	235	235	235	235
255	255	255	255	248	161	166	235	236	236	235	237	235	235
255	255	255	253	161	166	231	231	232	232	231	231	229	231
255	255	255	216	167	215	221	221	221	221	219	219	218	216
255	255	252	159	167	211	209	207	206	208	207	208	206	205
255	255	250	168	170	198	198	199	199	199	198	198	195	194
255	255	158	172	181	183	188	60	54	217	183	184	182	181
255	255	161	173	175	176	56	77	180	181	182	183	184	183
255	253	165	173	175	58	187	180	190	111	140	190	190	187
255	254	169	178	177	54	180	44	41	56	55	58	38	194
255	253	171	178	180	186	51	38	34	204	183	40	62	204
255	254	169	185	185	66	73	195	94	201	203	203	203	206
255	255	171	157	125	158	211	73	14	204	206	204	204	207
255	255	165	146	228	213	215	109	152	123	20	38	58	56

Image Matrix

Image Vector

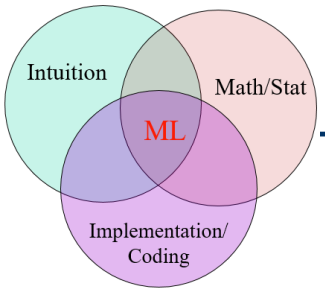
255 255 255 255 255 255 255 255 255 255 254 252 251 209 255 255 255 255 255 255 255 255 252 244 153 164 166 167 255 255 255 255 255 255 255 250 157 163 216 233 234 236

Machine learning

A major difference between the “modern machine learning” and “traditional artificial intelligence (AI)” fields is in the difference of data representations.

Machine learning: canonical numerical values. $\mathbb{R}$

Traditional AI: mixed raw inputs including continues, discrete, and categorical.



Recap: Supervised Learning

Intuition: A prediction task with a clear objective (e.g. a yes or no decision, which school to go to, a price to estimate, etc.) in which some history data for training can be acquired with the known prediction results already.

Math:

Training: $S_{training} = \{(\mathbf{x}_i, y_i), i = 1..n\}$

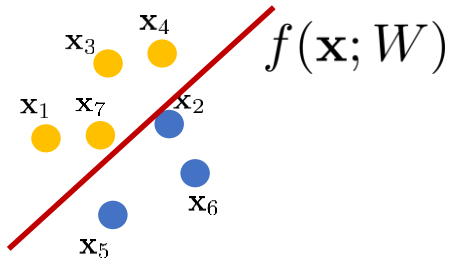
Testing: $S_{testing} = \{(\mathbf{x}_i), i = 1..u\}, what\ is\ y_i?$

Three key variables we are dealing with

Input: $\mathbf{x} = (x_1, x_2, ...)$

Label: $y \in 0, 1$

Model parameter: W



Features

Each data sample is often described by a set of features.

$\mathbf{x} = (x_1, x_2, ...)$

x_1: color
x_2 weight
...

Features are often multi-modality.

Three typical types:

1. Real number (continues), $x \in \mathbb{R}$.

   e.g. weight

2. Integer (continues), $x \in \mathbb{Z}$.

   e.g. age

3. Categorical (disjoint), $x \in \{red, blue, green, ...\}$.

   e.g. color

Feature representation

A major difference between the "modern machine learning" and "traditional artificial intelligence (AI)" fields is in the difference of data representations.

Machine learning: canonical numerical values. $\mathbb{R}$

Why do we care about creating a canonical feature representation?

Which of the following statements is FALSE?

A. To build generic mathematical formulations.
B. To scale up the learning/training process.
C. To build transparent machine learning algorithms.
D. To make different machine learning algorithms directly comparable.
E. To make a faster prediction in the testing time.

Feature representation

Why do we care about creating a canonical feature representation?

Which of the following statements is FALSE?

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D. To make different machine learning algorithms directly comparable.
E. To make a faster prediction in the testing time.

Mathematical representation for features

$$S = \{(\mathbf{x}_i), i = 1..n\} \qquad \mathbf{x}_i = (x_{i1}, ..., x_{im})$$

What if it is a city: $x_{i2} \in \{LosAngeles, SanDiego, Irvine\}$?

We ue a coding strategy by expanding the features.
For N number of possible states, we expand the features into N-dimenstional.

One-hot encoding:

	coded values
Los Angeles	1, 0, 0
San Diego	0, 1, 0
Irvine	0, 0, 1

Pros: we can naturally deal with any type of input (can associate confidence directly).

Cons: the feature dimension has become much larger.

One-hot encoding

- "One-hot encoding" is a standard technique that turns categorical features into general real numbers that can be used alone/together with other features in continues or discrete values.
- Feature values after one-hot encoding can take standard mathematical operations, just like standard real numbers.
- One-hot encoding can also generate soft values with a probabilistic interpretation, that is measurable and comparable.
- One-hot encoding gains in its convenience in a canonical mathematical representation by sacrificing in the space complexity: one category of k classes is turned into k real numbers in [0, 1].
- There are other encoding strategies, such as Word2Vec, that can turn categorical features into real numbers.

One-hot encoding

What if we simply:

	coded values
Los Angeles	1
San Diego	2
Irvine	3

This is wrong since it implies:

Los Angeles (1) + San Diego (2) = Irvine (3)

Irvin (3) > San Diego (2)

One-hot encoding with soft values

What if it is a city: $x_{i2} \in \{LosAngeles, SanDiego, Irvine\}$?

One-hot encoding:

	coded values		
70% Los Angeles and 30% San Diego	0.7,	0.3,	0
50% San Diego and 50% Irvine	0,	0.5,	0.5
Irvine	0,	0,	1

One-hot encoding

One-hot encoding with soft values

What if it is a city: $x_{i2} \in \{LosAngeles, SanDiego, Irvine\}$?

One-hot encoding:

	coded values		
70% Los Angeles and 30% San Diego	0.7,	0.3,	0
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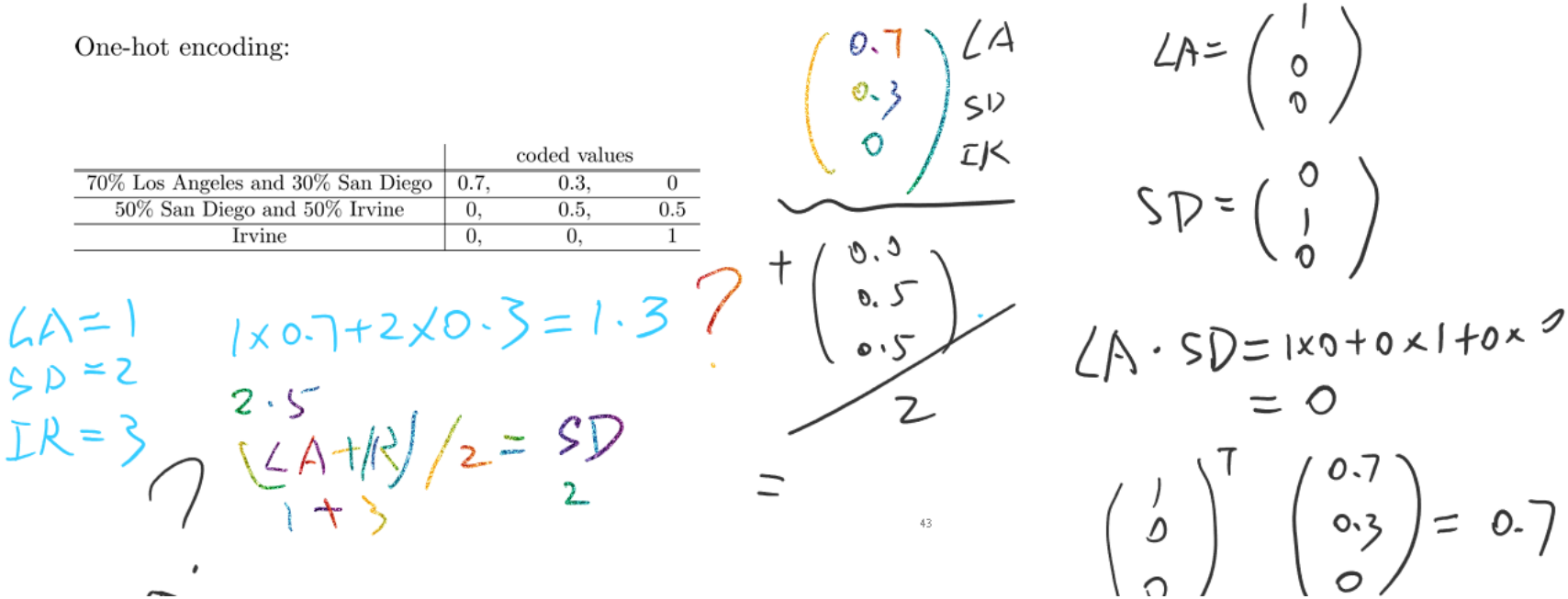


Data representation

$$S = \{\mathbf{x}_i, i = 1..n\} \qquad \mathbf{x}_i = (x_{i1}, ..., x_{im})$$

age	male or female	weight (lb)	height (cm)
$x_{11} = 22$	$x_{12} = M$	$x_{13} = 160$	$x_{14} = 180$
$x_{21} = 51$	$x_{22} = M$	$x_{23} = 190$	$x_{24} = 175$
$x_{31} = 43$	$x_{32} = F$	$x_{33} = 120$	$x_{34} = 165$

If we write each sample as a row vector:

$$\mathbf{x}_1 = (22, 0, 1, 160, 180)$$

$$X = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{pmatrix} \quad X \in \mathbb{R}^{n \times m}$$

$$X = \begin{pmatrix} 22 & 0 & 1 & 160 & 180 \\ 51 & 0 & 1 & 190 & 175 \\ 43 & 1 & 0 & 120 & 165 \end{pmatrix}$$

Data representation

$$S = \{\mathbf{x}_i, i = 1..n\} \qquad \mathbf{x}_i = (x_{i1}, ..., x_{im})^T$$

age	male or female	weight (lb)	height (cm)
$x_{11} = 22$	$x_{12} = M$	$x_{13} = 160$	$x_{14} = 180$
$x_{21} = 51$	$x_{22} = M$	$x_{23} = 190$	$x_{24} = 175$
$x_{31} = 43$	$x_{32} = F$	$x_{33} = 120$	$x_{34} = 165$

More often we write each sample as a COLUMN vector:

$$\mathbf{x}_1 = \begin{pmatrix} 22 \\ 0 \\ 1 \\ 160 \\ 180 \end{pmatrix}$$

$$X = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \quad X \in R^{m \times n}$$

$$X = \begin{pmatrix} 22 & 51 & 43 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \\ 160 & 190 & 120 \\ 180 & 175 & 165 \end{pmatrix}$$

Row or column vector?

$$\mathbf{x} = (22, 0, 1, 160, 180)$$

$$\mathbf{x} = \begin{pmatrix} 22 \\ 0 \\ 1 \\ 160 \\ 180 \end{pmatrix}$$

row vector

column vector

$$\mathbf{w} = (w_1, w_2, w_3, w_4, w_5)$$

$$\mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{pmatrix}$$

$$\mathbf{w} \cdot \mathbf{x} \equiv < \mathbf{w}, \mathbf{x} > \equiv \mathbf{w}\mathbf{x}^T$$

$$\mathbf{w} \cdot \mathbf{x} \equiv < \mathbf{w}, \mathbf{x} > \equiv \mathbf{w}^T\mathbf{x}$$

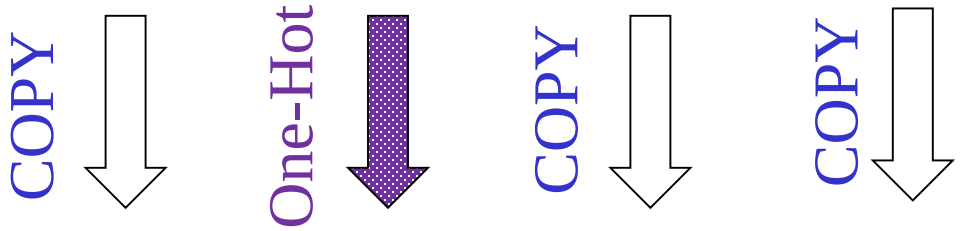
Row vector or column vector can be alternatively used, but make sure you stick to the same definition/setting in your problem formulations.

It is slightly more common to use the column vector representation:

Building a canonical mathematical representation

age	male or female	weight (lb)	height (cm)
$x_{11} = 22$	$x_{12} = M$	$x_{13} = 160$	$x_{14} = 180$
$x_{21} = 51$	$x_{22} = M$	$x_{23} = 190$	$x_{24} = 175$
$x_{31} = 43$	$x_{32} = F$	$x_{33} = 120$	$x_{34} = 165$

discrete categorical continues continues



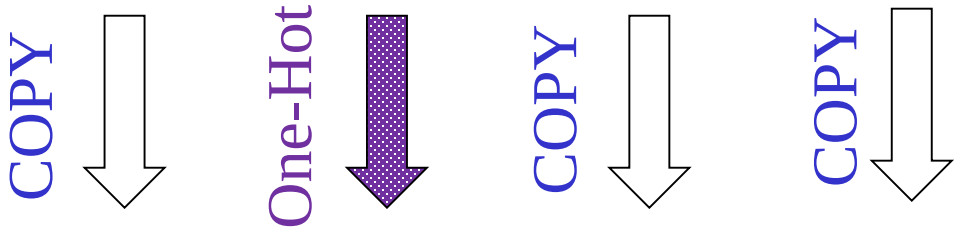
$$\begin{pmatrix} 22 & 0 & 1 & 160 & 180 \\ 51 & 0 & 1 & 190 & 175 \\ 43 & 1 & 0 & 120 & 165 \end{pmatrix}$$

Building a canonical mathematical representation

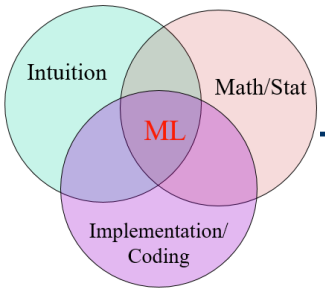
For a categorical feature that has only two possible categories, we sometimes use only one entry to reduce the encoded feature size.

age	male or female	weight (lb)	height (cm)
$x_{11} = 22$	$x_{12} = M$	$x_{13} = 160$	$x_{14} = 180$
$x_{21} = 51$	$x_{22} = M$	$x_{23} = 190$	$x_{24} = 175$
$x_{31} = 43$	$x_{32} = F$	$x_{33} = 120$	$x_{34} = 165$

discrete categorical continues continues



$$\begin{pmatrix} 22 & 0 & 160 & 180 \\ 51 & 0 & 190 & 175 \\ 43 & 1 & 120 & 165 \end{pmatrix}$$



Recap: One-hot Encoding

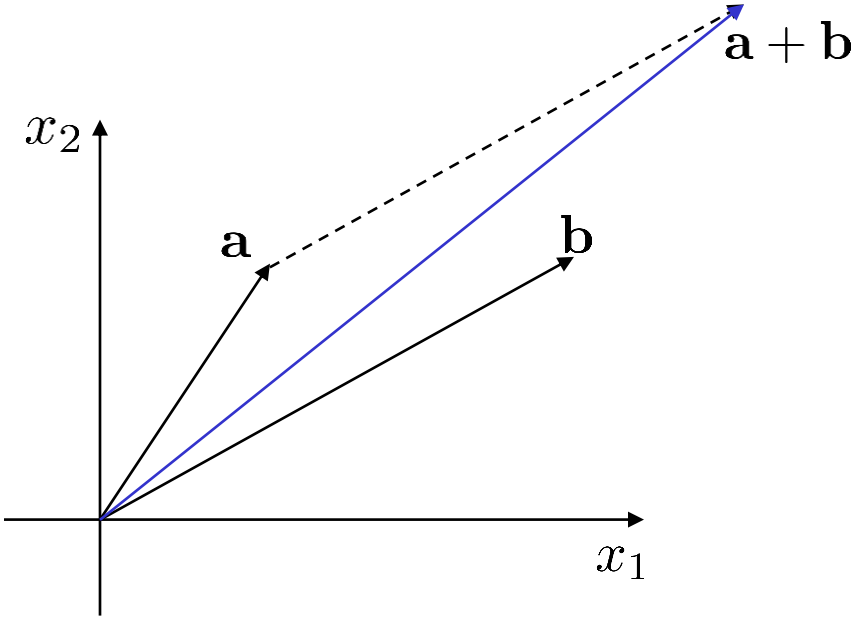
Intuition: Turn categorical features (e.g. city, school, name, etc.) to which arithmetic operations cannot be applied into real numbers for direct mathematical manipulations. After the transformation, the input features originally described as categories have no difference to those in real numbers. They will be treated canonically in the later mathematical and statistical functions.

Math: $x_{raw} \in \{Los\ Angeles, San\ Diego, Irvine\}$

category	$\mathbf{x}_{one-hot}$
Los Angeles	1, 0, 0
San Diego	0, 1, 0
Irvine	0, 0, 1

Vector

Addition:



$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

$$\mathbf{a}+\mathbf{b} = \begin{pmatrix} a_1+b_1 \\ a_2+b_2 \\ a_3+b_3 \end{pmatrix}$$

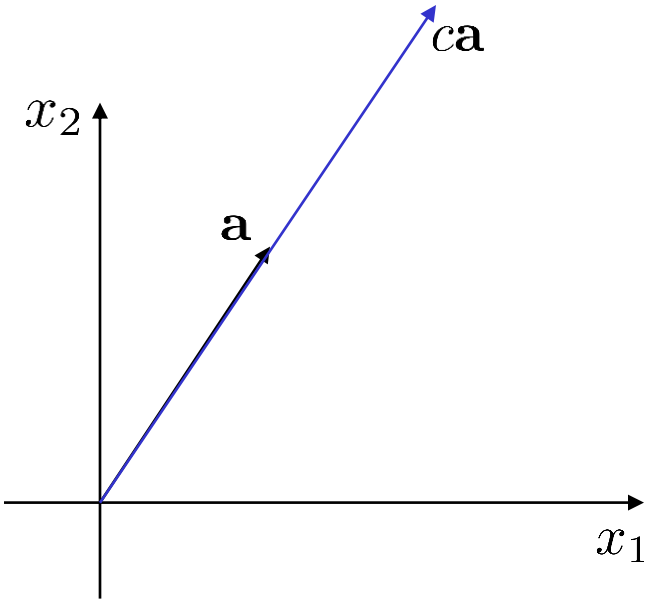
It's still a vector in the same space as a and b.

Visual illustration by 3Blue1Brown

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

Vector

Scaling:



$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$c \in R$$

$$c\mathbf{a} = \begin{pmatrix} c \times a_1 \\ c \times a_2 \\ c \times a_3 \end{pmatrix}$$

It's still a vector in the same space as a.

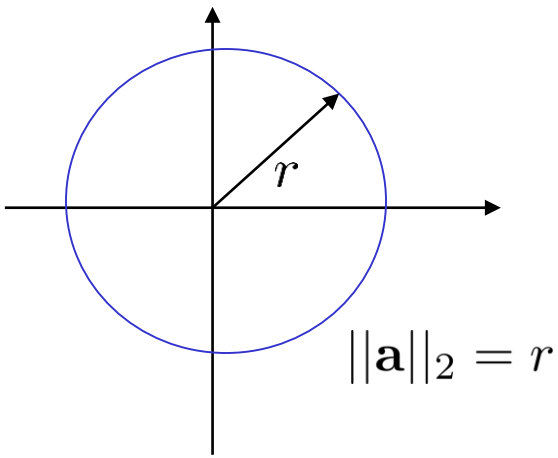
Norm

$\mathbf{a} = (a_1, a_2, ..., a_n),\ a_i \in \mathbb{R}$

L2 Norm:

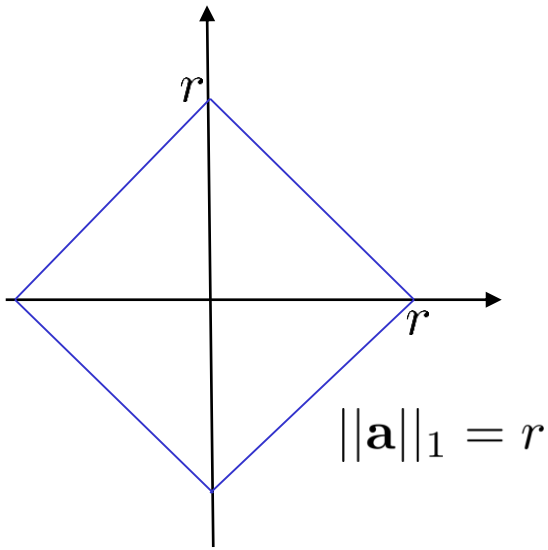
$$||\mathbf{a}||_2 = \sqrt{\sum_{i=1}^{n} a_i^2}$$

$$||\mathbf{a}||_2^2 = \sum_{i=1}^{n} a_i^2$$



L1 Norm:

$$||\mathbf{a}||_1 = \sum_{i=1}^{n} |a_i|$$



Norm

$$||\mathbf{a}||_2 = \sqrt{\sum_{i=1}^{n} a_i^2}$$

We use norm (typically L2) to measure the "length" (magnitude) of a vector.

Norm is a non-negative real number (scalar).

In machine learning,

1. we sometimes use norm to normalize an in put vector,

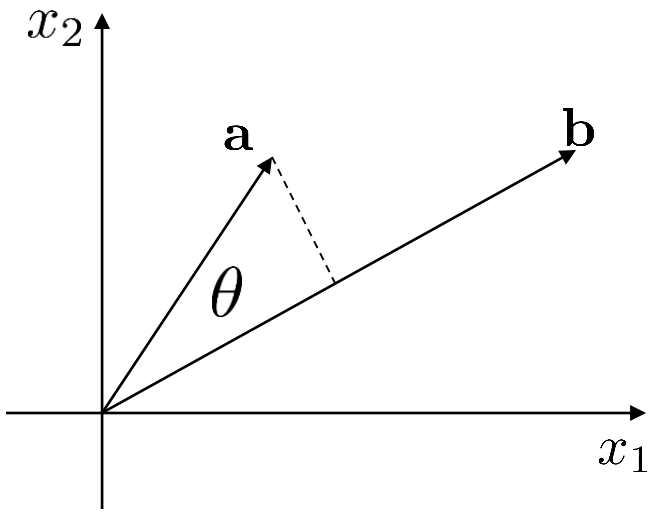
   $\mathbf{a}/||\mathbf{a}||_2$

2. or to use norm as a regularization to prevent overfitting for the model parameter

   $||\mathbf{w}||_2$

Vector: Projection (inner product)

(one of the most important concepts in machine learning)



$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

$$< \mathbf{a}, \mathbf{b} > \equiv \mathbf{a} \cdot \mathbf{b} \equiv \mathbf{a}^T \mathbf{b} \equiv a_1 b_1 + a_2 b_2 + a_3 b_3$$

It's a scalar!

$$cos(\theta) = \frac{<\mathbf{a},\mathbf{b}>}{||\mathbf{a}||_2 \times ||\mathbf{b}||_2}$$

Significance of the dot product between two vectors

"Dot product" outputs a scalar value and it is arguably the most important mathematical operation in machine learning.

$$< \mathbf{a}, \mathbf{b} > \equiv \mathbf{a} \cdot \mathbf{b} \equiv \mathbf{a}^T \mathbf{b}$$
$$\equiv < \mathbf{b}, \mathbf{a} > \equiv \mathbf{b} \cdot \mathbf{a} \equiv \mathbf{b}^T \mathbf{a}$$

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

Why?

"Dot product" computes for the magnitude for the projection from one vector to the other, which essentially measures the "similarity" between two vectors.

For two unit vectors (L2 norm being 1), their dot product outputs the largest value 1 when they well aligned (same), and otherwise 0 when they are orthogonal (different) to each other.

Significance of the dot product between two vectors

	fly?	laying eggs?	weight (lb)
sparrow	yes	yes	0.087
chipmunk	no	no	0.19
bat	yes	no	0.09

Feature representation (one-hot encoded).

$$\text{sparrow} = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0.087 \end{pmatrix} \qquad \text{chipmunk} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0.19 \end{pmatrix} \qquad \text{bat} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0.09 \end{pmatrix}$$

$\text{sparrow} \cdot \text{chipmunk} = 0.01653$ very different!

$\text{sparrow} \cdot \text{bat} = 1.00783$

$\text{chipmunk} \cdot \text{bat} = 1.0171$

More illustrations about vector operations

https://www.youtube.com/watch?v=fNk_zzaMoSs&t=3s

3Blue1Brown

Basics about data and linear algebra operations

$$S = \{(\mathbf{x}_i, y_i), i = 1..n\} \qquad y_i \in \{-1, +1\}$$

	age	male or female	weight (lb)	height (cm)
$y_1 = -1$ (negative)	$x_{11} = 22$	$x_{12} = M$	$x_{13} = 160$	$x_{14} = 180$
$y_2 = +1$ (positive)	$x_{21} = 51$	$x_{22} = M$	$x_{23} = 190$	$x_{24} = 175$
$y_3 = +1$ (positive)	$x_{31} = 43$	$x_{32} = F$	$x_{33} = 120$	$x_{34} = 165$

$$X = \begin{pmatrix} 22 & 1 & 0 & 160 & 180 \\ 51 & 1 & 0 & 190 & 175 \\ 43 & 0 & 1 & 120 & 165 \end{pmatrix} \qquad Y = \begin{pmatrix} -1 \\ +1 \\ +1 \end{pmatrix}$$

$$W = \begin{pmatrix} 0.075 \\ 0 \\ 0 \\ -0.007 \\ -0.008 \end{pmatrix} \qquad \hat{Y} = XW = \begin{pmatrix} -0.91 \\ 1.095 \\ 1.065 \end{pmatrix}$$

Matrix multiplication

Vector:

$$A = \begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix} \qquad B = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

$$AB = \begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = a_1 b_1 + a_2 b_2 + a_3 b_3$$

$$AB \neq BA$$

$$BA = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix} = \begin{pmatrix} b_1 a_1 & b_1 a_2 & b_1 a_3 \\ b_2 a_1 & b_2 a_2 & b_2 a_3 \\ b_3 a_1 & b_3 a_2 & b_3 a_3 \end{pmatrix}$$

Matrix multiplication

Matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} \qquad B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{pmatrix}$$

$$AB = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{pmatrix}$$

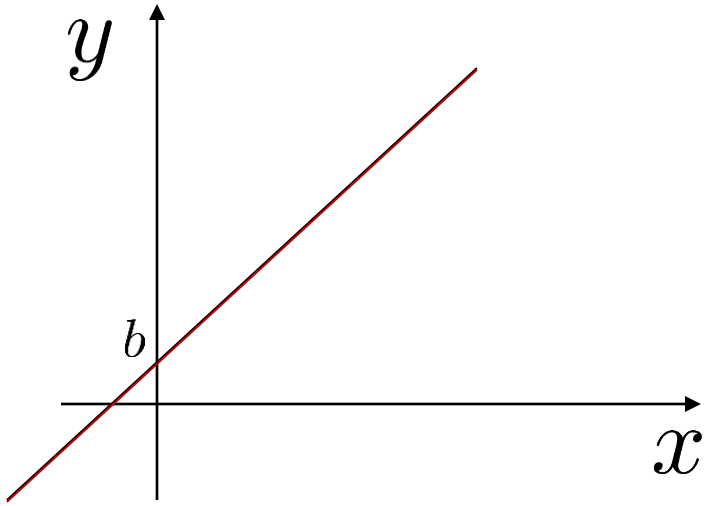
$$= \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} & a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} & a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} \end{pmatrix}$$

Calculus

Scalar:

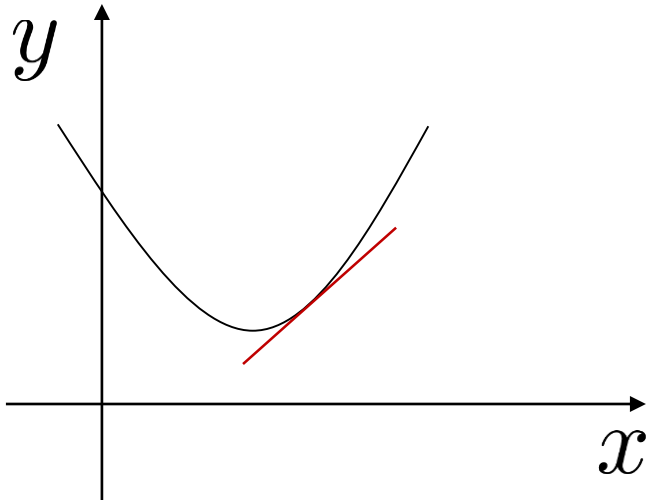
$$y = ax + b$$

$$\frac{dy}{dx} = a$$



$$y = ax^2 + bx + c$$

$$\frac{dy}{dx} = 2ax + b$$



Vector calculus

Vector derivatives

Vector-by-scalar

$$\mathbf{y}(x) = \begin{pmatrix} y_1(x) & y_2(x) & y_3(x) \end{pmatrix}$$

$$\frac{d\mathbf{y}(x)}{dx} = \begin{pmatrix} \frac{dy_1(x)}{dx} & \frac{dy_2(x)}{dx} & \frac{dy_3(x)}{dx} \end{pmatrix}$$

Vector-by-vector

$$\mathbf{y}(\mathbf{x}) = \begin{pmatrix} y_1(\mathbf{x}) & , \ldots, & y_m(\mathbf{x}) \end{pmatrix}$$

$$\mathbf{x} = \begin{pmatrix} x_1 & , \ldots, & x_n \end{pmatrix}$$

$$\frac{d\mathbf{y}(\mathbf{x})}{d\mathbf{x}} = \begin{pmatrix} \frac{dy_1(\mathbf{x})}{dx_1} & , \ldots, & \frac{dy_m(\mathbf{x})}{dx_1} \\ . & . & . \\ \frac{dy_1(\mathbf{x})}{dx_n} & , \ldots, & \frac{dy_m(\mathbf{x})}{dx_n} \end{pmatrix}$$

Vector calculus

Vector-by-vector

$$A = \begin{pmatrix} a_{11} & , \ldots, & a_{1m} \\ . & . & . \\ a_{n1} & , \ldots, & a_{nm} \end{pmatrix}$$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ . \\ x_m \end{pmatrix}$$

$$\frac{\partial A\mathbf{x}}{\partial \mathbf{x}} = A$$

numerator form

$$\frac{\partial \mathbf{x}^T A^T}{\partial \mathbf{x}} = A$$

denominator form

Vector calculus

Identities: vector-by-vector $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$

Condition	Expression	Numerator layout, i.e. by y and $\mathbf{x}^\mathsf{T}$	Denominator layout, i.e. by $\mathbf{y}^\mathsf{T}$ and x
a is not a function of **x**	$\frac{\partial \mathbf{a}}{\partial \mathbf{x}} =$	$\mathbf{0}$	
	$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{I}$	
A is not a function of **x**	$\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{A}$	$\mathbf{A}^\top$
A is not a function of **x**	$\frac{\partial \mathbf{x}^\top \mathbf{A}}{\partial \mathbf{x}} =$	$\mathbf{A}^\top$	$\mathbf{A}$
a is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	
a = *a*(**x**), **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}\frac{\partial a}{\partial \mathbf{x}}$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial a}{\partial \mathbf{x}}\mathbf{u}^\top$
A is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial \mathbf{A}\mathbf{u}}{\partial \mathbf{x}} =$	$\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}^\top$
u = **u**(**x**), **v** = **v**(**x**)	$\frac{\partial (\mathbf{u}+\mathbf{v})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$	
u = **u**(**x**)	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}$

https://en.wikipedia.org/wiki/Matrix_calculus

Why is computing the vector derivatives so important?

Which statement is NOT true?

A. Help us better understand the machine learning problem.

B. Can always be accurately computed.

C. Gives a principled and general way for training a machine learning algorithm.

D. Scales up to big high-dimensional data.

Why is computing the vector derivatives so important?

Which statement is NOT true?

A. Help us better understand the machine learning problem.

☆B. Can always be accurately computed.

C. Gives a principled and general way for training a machine learning algorithm.

D. Scales up to big high-dimensional data.

Matrix calculus

Matrix-by-scalar

$$Y(x) = \begin{pmatrix} y_{11}(x) & , \ldots, & y_{1m}(x) \\ . & . & . \\ y_{n1}(x) & , \ldots, & y_{nm}(x) \end{pmatrix}$$

$$\frac{dY(x)}{dx} = \begin{pmatrix} \frac{dy_{11}(x)}{dx} & , \ldots, & \frac{dy_{1m}(x)}{dx} \\ \frac{dy_{n1}(x)}{dx} & , \ldots, & \frac{dy_{nm}(x)}{dx} \end{pmatrix}$$

Matrix calculus

Scalar-by-vector

$$A = \begin{pmatrix} a_{11} & , \ldots, & a_{1n} \\ . & . & . \\ a_{n1} & , \ldots, & a_{nn} \end{pmatrix}$$

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

$$\frac{\partial \mathbf{x}^T A \mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{x}^T A$$

Matrix calculus

Condition	Expression	Numerator layout, i.e. by x^T; result is row vector	Denominator layout, i.e. by x; result is column vector
a is not a function of **x**	$\frac{\partial(\mathbf{a}\cdot\mathbf{x})}{\partial\mathbf{x}} = \frac{\partial(\mathbf{x}\cdot\mathbf{a})}{\partial\mathbf{x}} =$ $\frac{\partial\mathbf{a}^\top\mathbf{x}}{\partial\mathbf{x}} = \frac{\partial\mathbf{x}^\top\mathbf{a}}{\partial\mathbf{x}} =$	$\mathbf{a}^\top$	$\mathbf{a}$
A is not a function of **x** **b** is not a function of **x**	$\frac{\partial\mathbf{b}^\top\mathbf{A}\mathbf{x}}{\partial\mathbf{x}} =$	$\mathbf{b}^\top\mathbf{A}$	$\mathbf{A}^\top\mathbf{b}$
A is not a function of **x**	$\frac{\partial\mathbf{x}^\top\mathbf{A}\mathbf{x}}{\partial\mathbf{x}} =$	$\mathbf{x}^\top(\mathbf{A}+\mathbf{A}^\top)$	$(\mathbf{A}+\mathbf{A}^\top)\mathbf{x}$
A is not a function of **x** **A** is symmetric	$\frac{\partial\mathbf{x}^\top\mathbf{A}\mathbf{x}}{\partial\mathbf{x}} =$	$2\mathbf{x}^\top\mathbf{A}$	$2\mathbf{A}\mathbf{x}$
A is not a function of **x**	$\frac{\partial^2\mathbf{x}^\top\mathbf{A}\mathbf{x}}{\partial\mathbf{x}^2} =$	$\mathbf{A}+\mathbf{A}^\top$	
A is not a function of **x** **A** is symmetric	$\frac{\partial^2\mathbf{x}^\top\mathbf{A}\mathbf{x}}{\partial\mathbf{x}^2} =$	$2\mathbf{A}$	

https://en.wikipedia.org/wiki/Matrix_calculus

Vector and Matrix Calculus

The main reason to study/use vector calculus is to formulate machine learning problems using canonical mathematical representations that can be accepted by the generic machine learning algorithms including neural networks, decision tree, nearest neighborhood, boosting, logistic regression classifier etc.

Using vector representations with vector calculus significantly facilitates the understanding, training, evaluating, scaling up, and transferring of the machine learning algorithms with significantly reduced overhead and customization.

Vector and Matrix Calculus

One way to master the concept of vector representation and calculus is by simplifying (conceptually) the formulation into scalar cases, which can be understood more easily.

Taking the derivatives w.r.t. scalar and vector gives us a strong leverage in using vector calculus for performing optimization to train the various machine learning algorithms.