Data, Model and Loss

Alexander Jung
Assistant Professor for Machine Learning
Department of Computer Science
Aalto University

Learning Goals

- develop intuition for how ML works
- become familiar with concept of data points
- ...with concept of a model
- ...with concept of a loss function

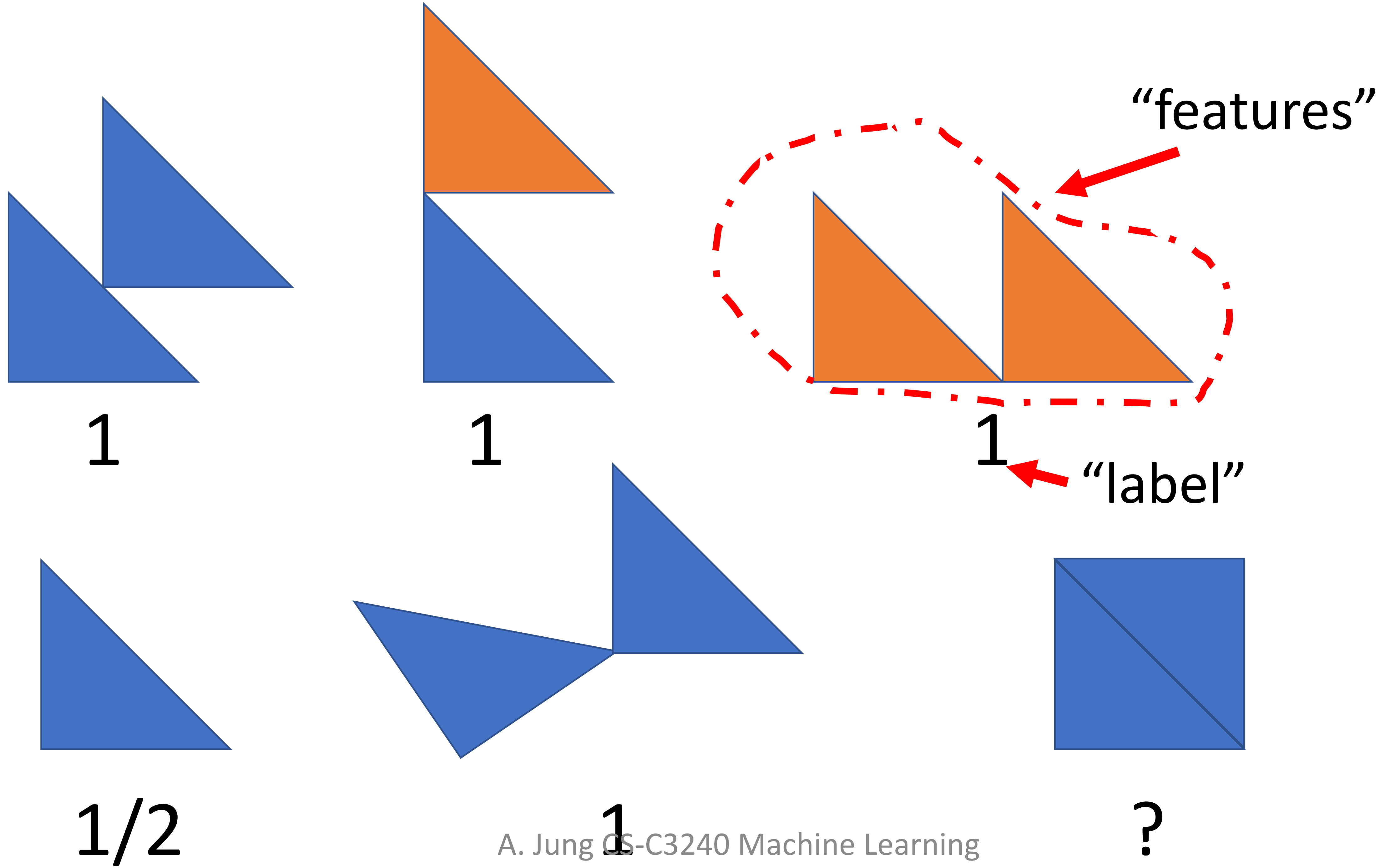
What is all About ?

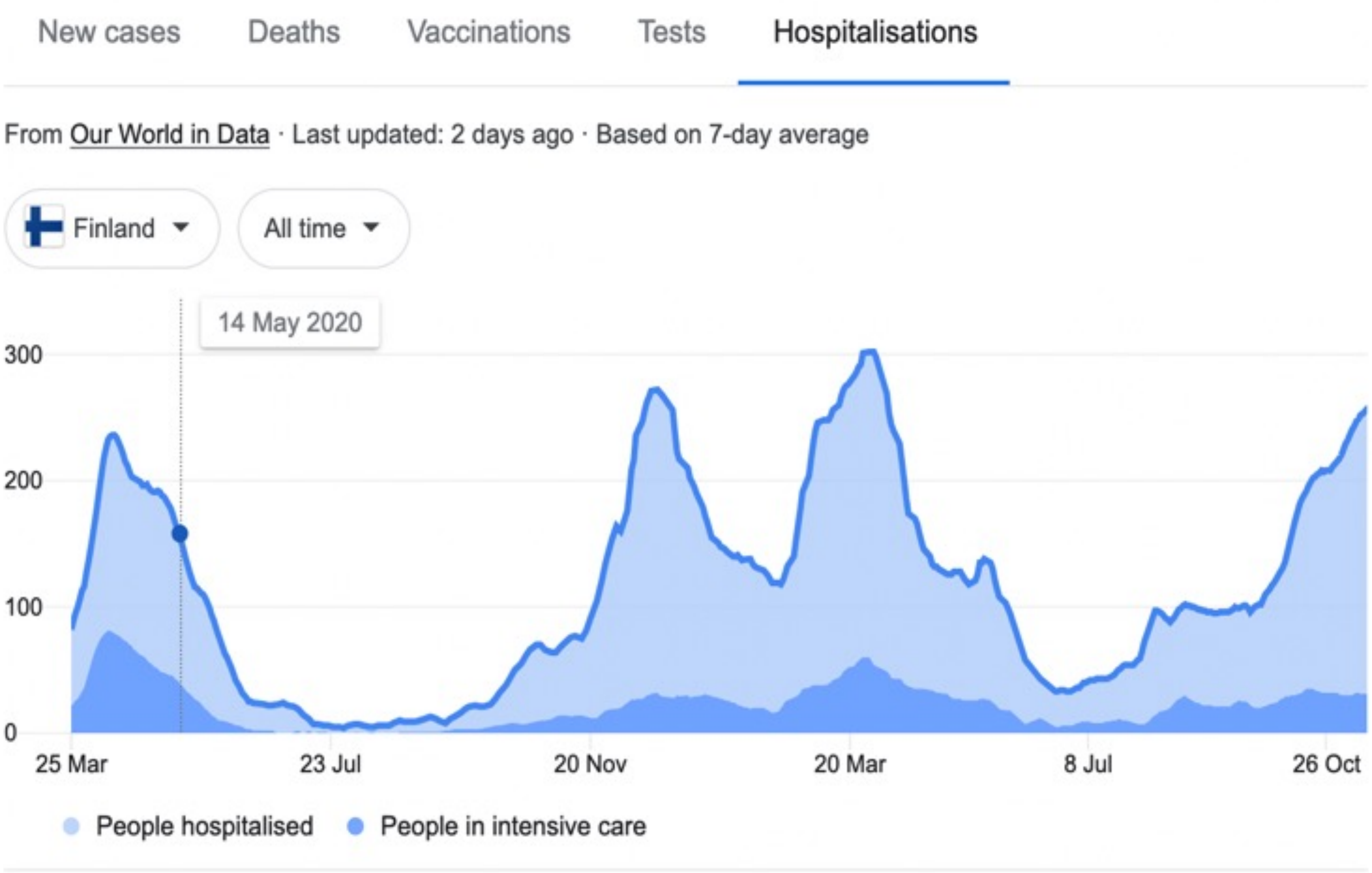
fit models to data to make

predictions or forecasts !

1. element	2.	3.	4.	5.	6.
4,	5,	6,	7,	8,	?

"data point"

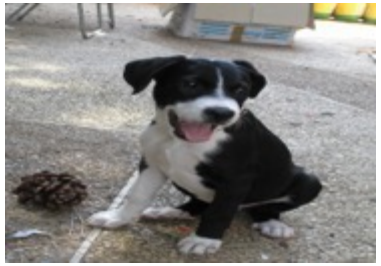

“features”
1
1
1
“label”
1/2
1
?


New cases
Deaths
Vaccinations
Tests
Hospitalisations
From Our World in Data · Last updated: 2 days ago · Based on 7-day average
Finland
All time
14 May 2020
300
200
100
0
25 Mar
23 Jul
20 Nov
20 Mar
8 Jul
26 Oct
People hospitalised
People in intensive care

?

?

features (pixel RGB values)



"Cat" "Dog" "Cat" ?

label

https://commons.wikimedia.org/

“feature”

min tmp: -10
max tmp: -3

min tmp: -3
max tmp: 4

min tmp: 1
max tmp: 5

data point

min tmp: -6
max tmp: ?

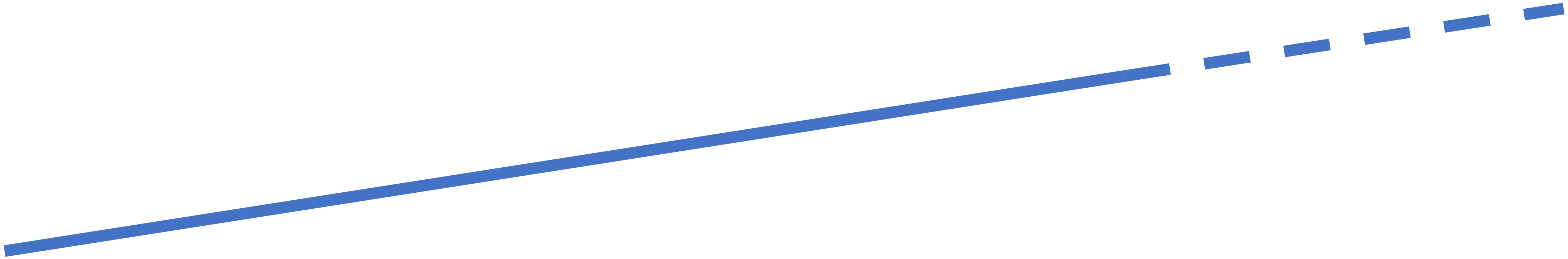
“label”

so, how does it work?

use hypothesis about data generation

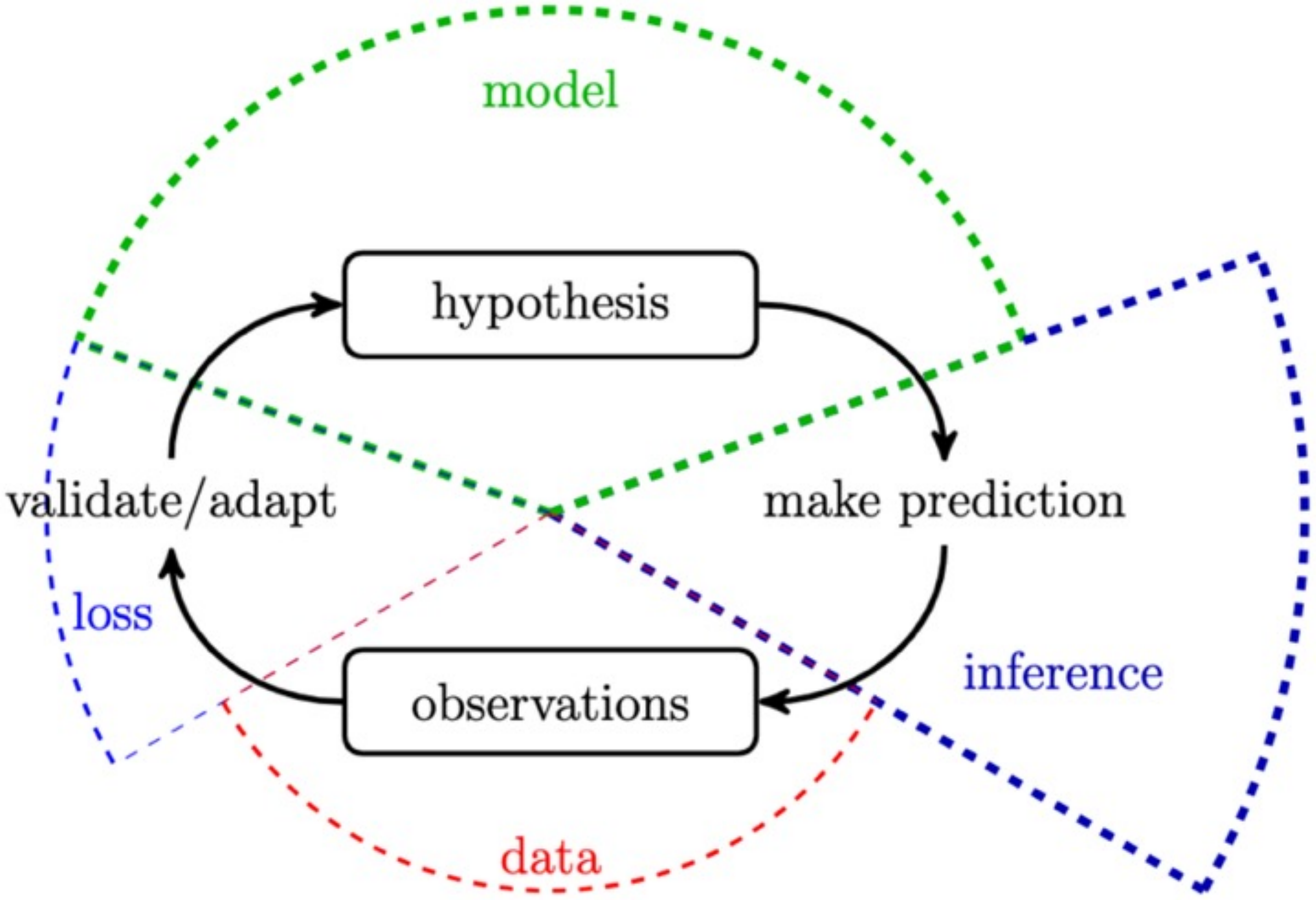
to make predictions (forecasts)

4, 5, 6, 7, 8, ?

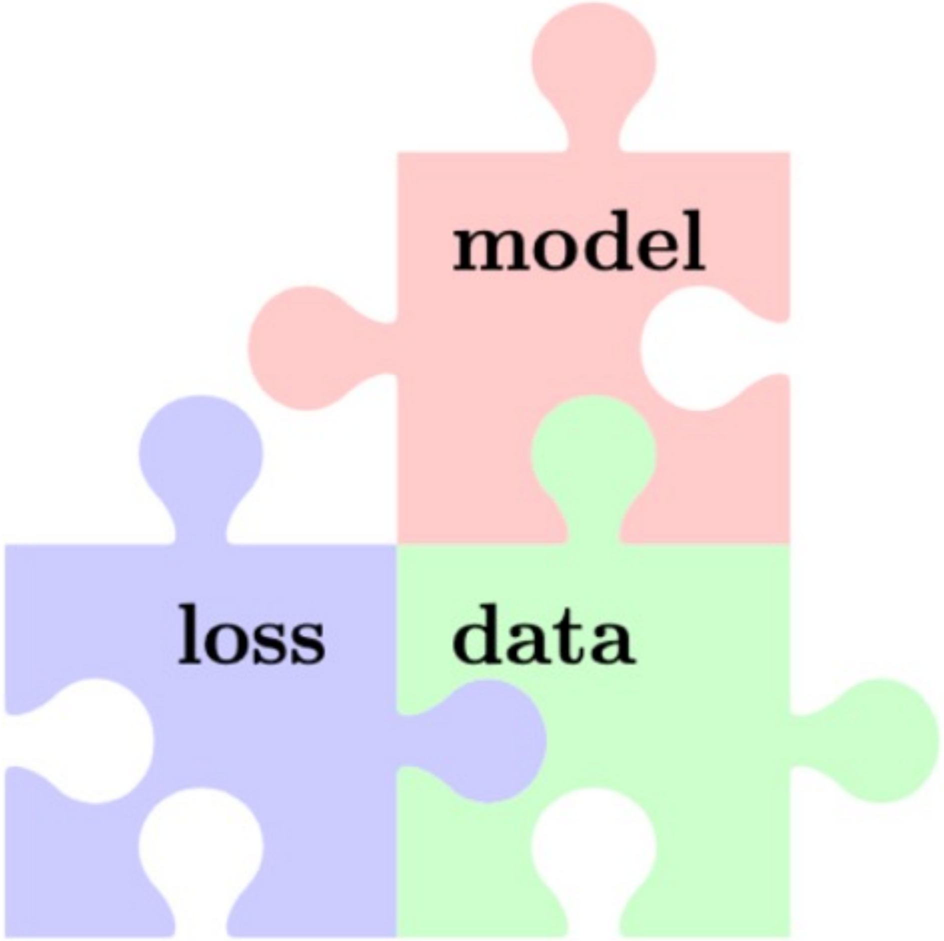


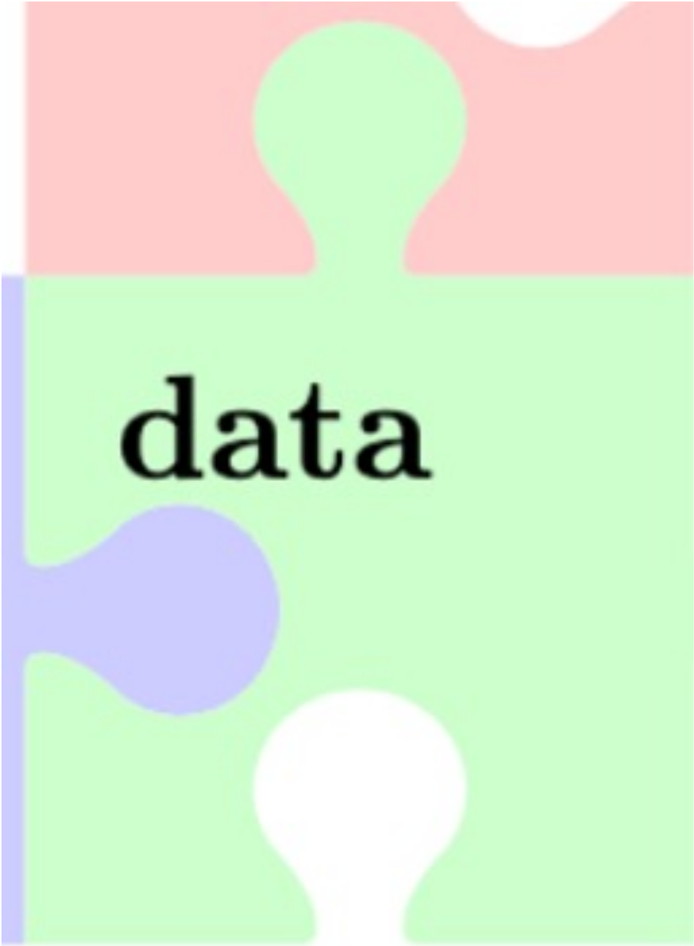
“hypothesis”

“Life-Long Learning”



Three Components of ML





"What I'm finding is that for a lot of problems, it'd be useful to shift our mindset toward not just improving the code but in a more systematic way of improving the data," said Andrew Ng

https://read.deeplearning.ai/the-batch/issue-84/

data

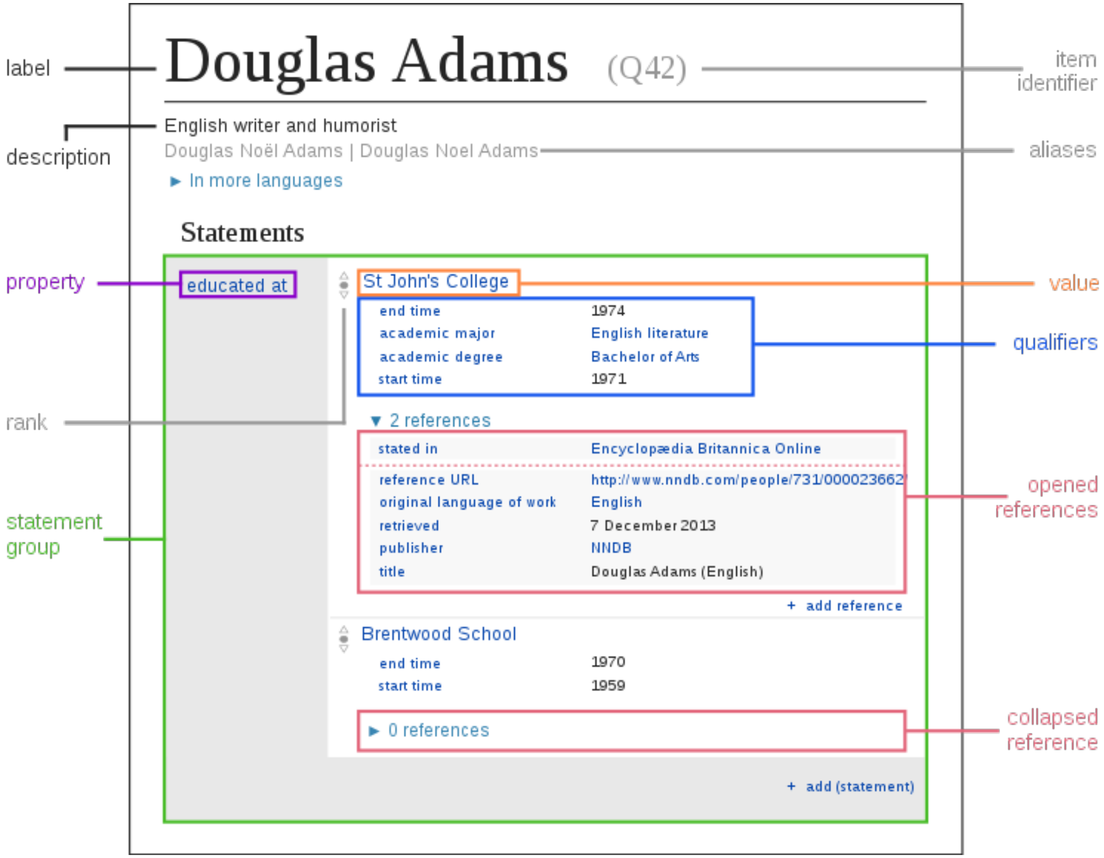
=

set of datapoints

What is a Datapoint?

some object that might carry relevant information

Datapoint = Some Item in Wikidata

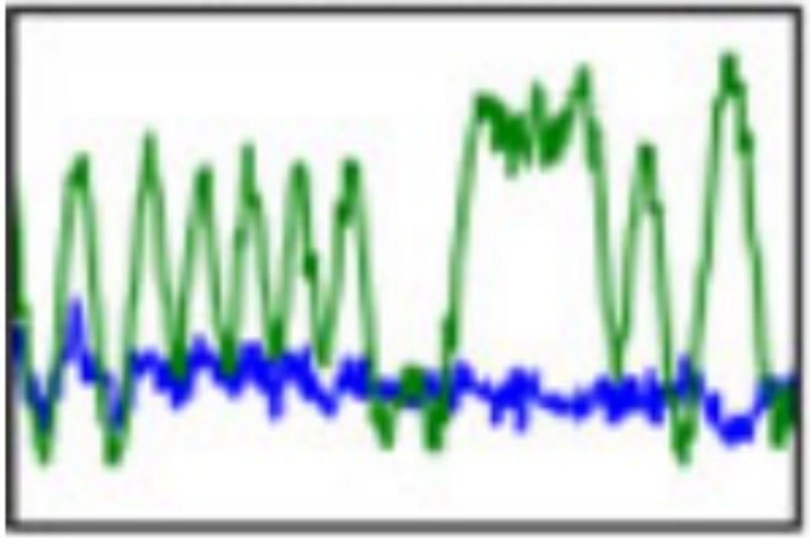


https://upload.wikimedia.org/wikipedia/commons/a/ae/Datamodel_in_Wikidata.svg

Datapoint = Some Period of Time

1.1.2020 01:00 - 2.1.2020 13:00

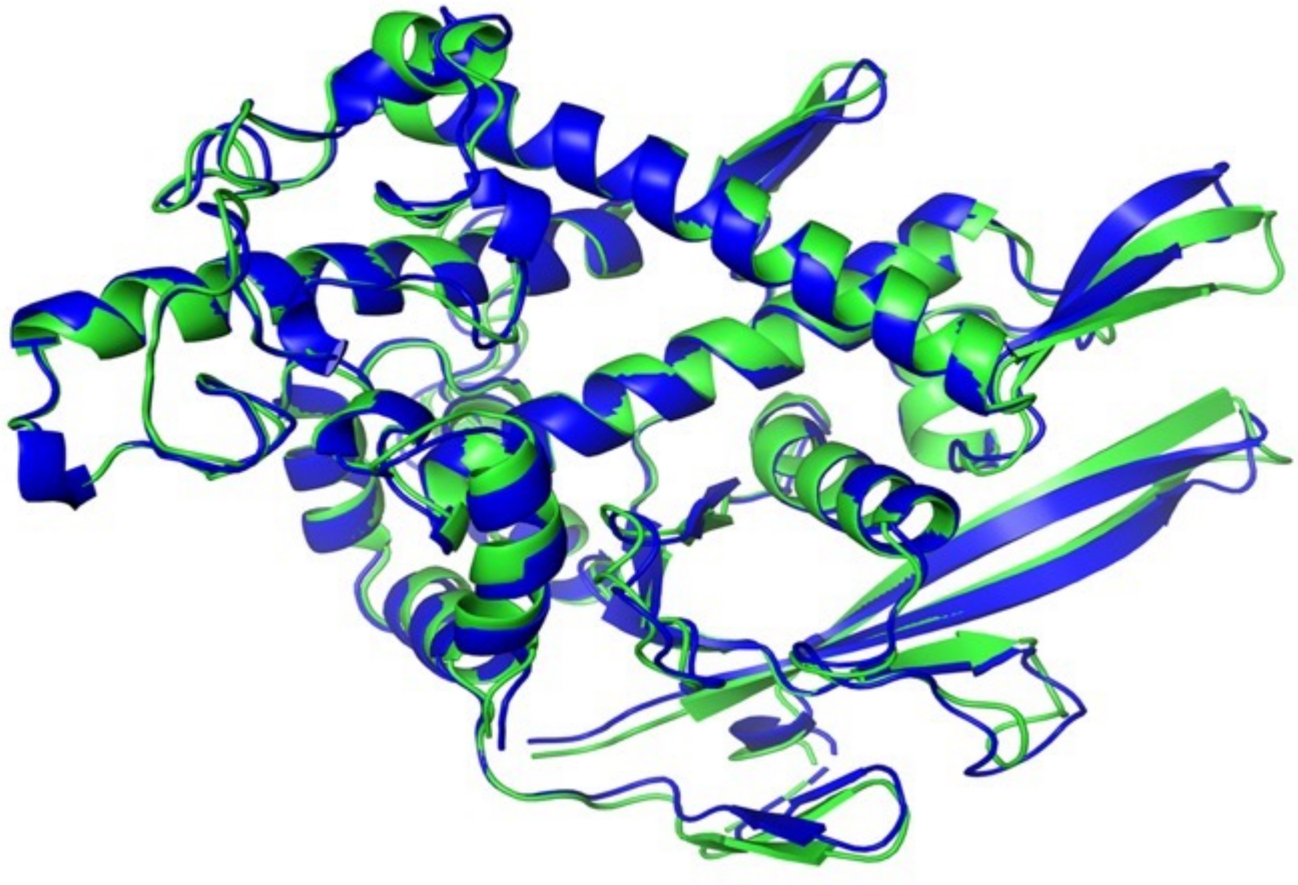
Datapoint = Some Wireless Signal



T. J. O’Shea, T. Roy and T. C. Clancy,
"Over-the-Air Deep Learning Based Radio Signal Classification,"
in *IEEE Journal of Selected Topics in Signal Processing*, vol. 12, no. 1, pp. 168-179, Feb. 2018,
doi: 10.1109/JSTSP.2018.2797022.

Datapoint = Some Country

Datapoint = Some Protein



Datapoint = A Partial Differential Equation

$$\frac{\partial u}{\partial t}(t,x) + \frac{1}{2}\mathrm{Tr}\left(\sigma\sigma^{\mathrm{T}}(t,x)(\mathrm{Hess}_x u)(t,x)\right) + \nabla u(t,x)\cdot\mu(t,x)$$
$$+ f\left(t,x,u(t,x),\sigma^{\mathrm{T}}(t,x)\nabla u(t,x)\right) = 0 \qquad \mathbf{[1]}$$

RESEARCH ARTICLE

Solving high-dimensional partial differential equations using deep learning

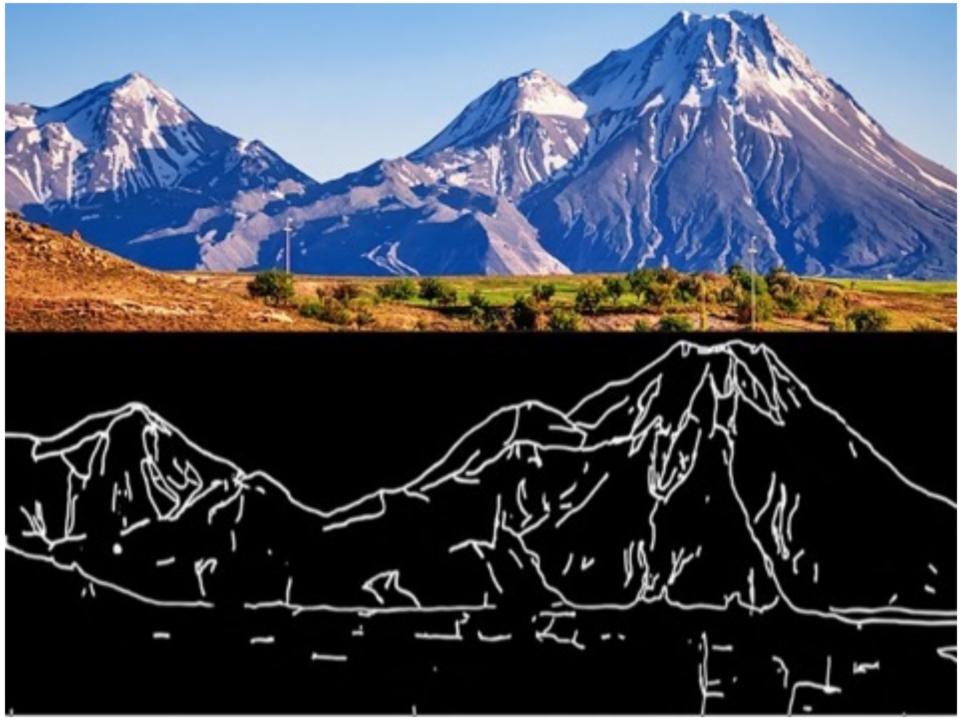
Jiequn Han, Arnulf Jentzen, and Weinan E
+ See all authors and affiliations

https://www.pnas.org/content/115/34/8505/tab-article-info

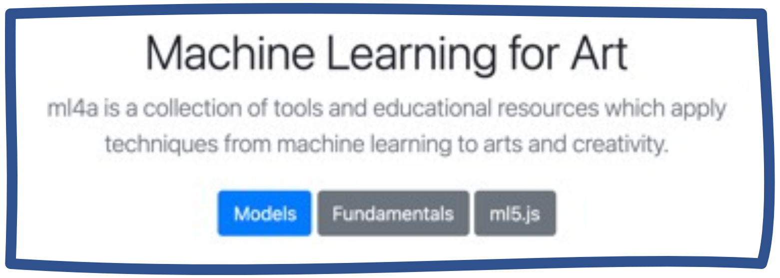
Datapoint = Some Bridge

https://commons.wikimedia.org/wiki/Category:Bridges

Datapoint = Image Sketch



https://ml4a.net/



Features and Labels.

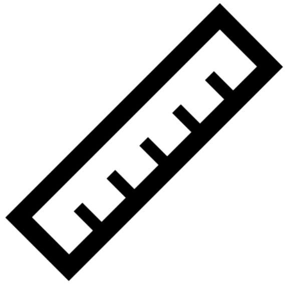
datapoint characterized by

- features: low-level properties; easy to measure/compute

- labels: high-level quantity of interest; difficult to measure/determine

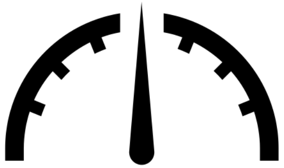
Numeric Features

we mainly use numeric features
x1,…,xn to characterize a datapoint



stack features into feature vector

Python: use numpy array to store features



discuss feature learning methods later

Features of an Image.

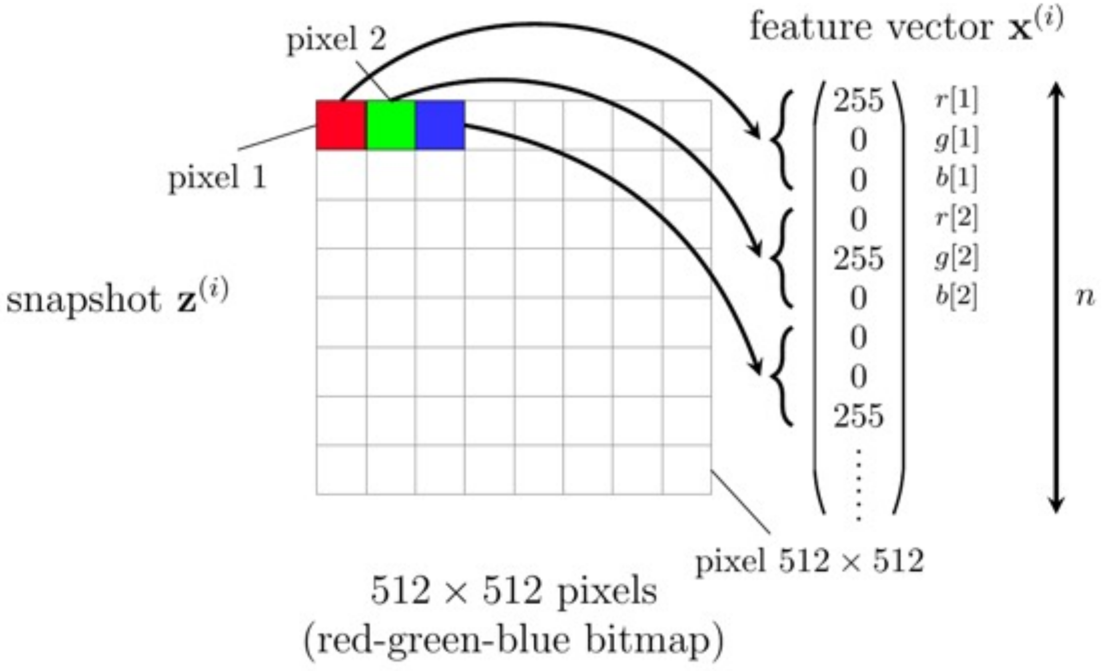


Figure 2.5: If the snapshot $\mathbf{z}^{(i)}$ is stored as a 512×512 RGB bitmap, we could use as features $\mathbf{x}^{(i)} \in \mathbb{R}^n$ the red-, green- and blue component of each pixel in the snapshot. The length of the feature vector would then be $n = 3 \times 512 \times 512 \approx 786000$.

Features of an Audio Recording.

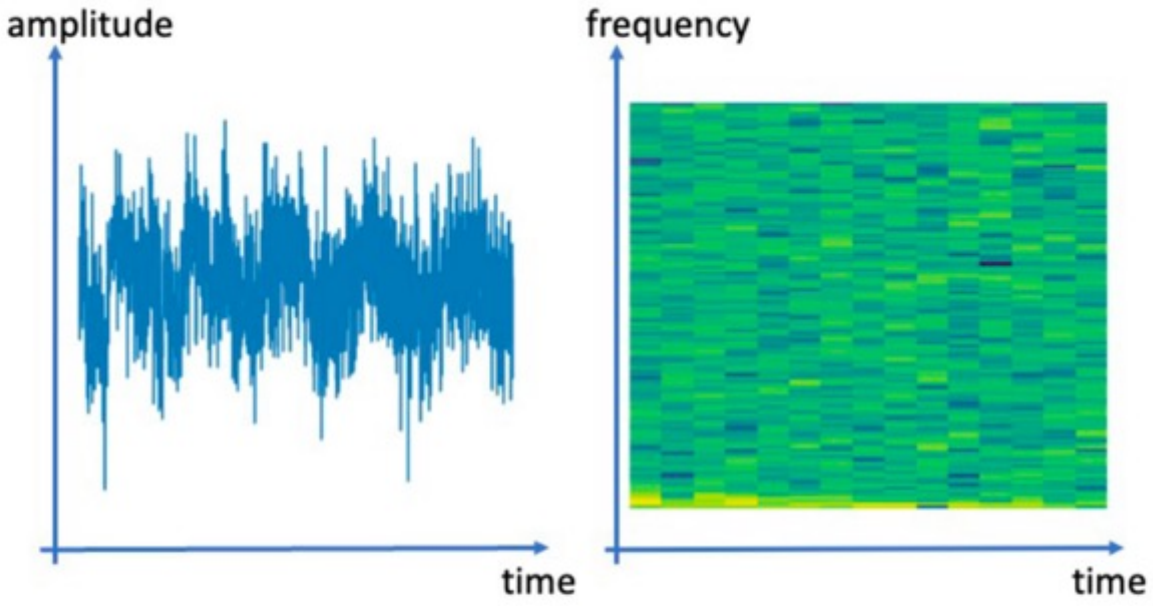


Figure 2.4: Two visualizations of a data point that represents an audio recording. The left figure shows a line plot of the audio signal amplitudes. The right figure shows a spectogram of the audio recording.

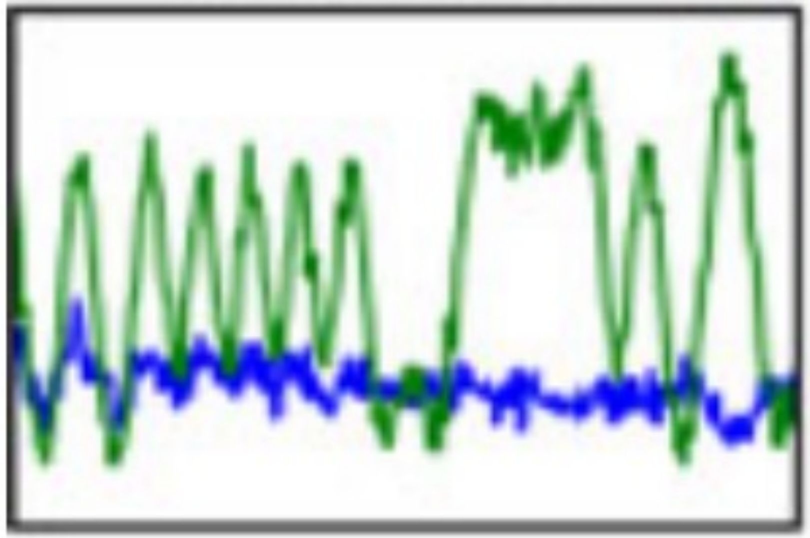
Datapoint = Period of Time

$\boxed{\text{1.1.2020 00:00 - 1.1.2020 23:55}}$

features: temperature recordings @ 01:00, 03:00, 05:00

label: temperature recording @ 23:00

Datapoint = Wireless Signal

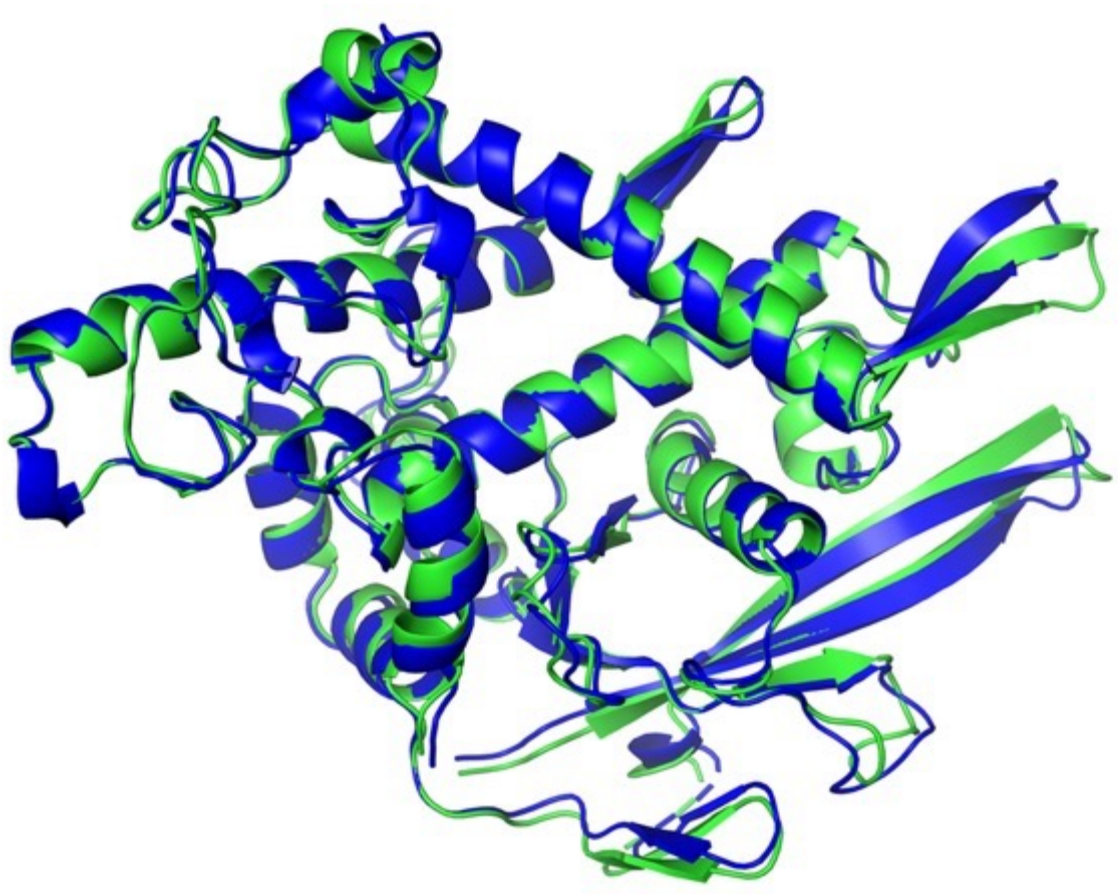


features:

label:

T. J. O’Shea, T. Roy and T. C. Clancy,
"Over-the-Air Deep Learning Based Radio Signal Classification,"
in *IEEE Journal of Selected Topics in Signal Processing*, vol. 12, no. 1, pp. 168-179, Feb. 2018,
doi: 10.1109/JSTSP.2018.2797022.

Datapoint = A Protein



features:

label:

Datapoint = A Partial Differential Equation

$$\frac{\partial u}{\partial t}(t,x) + \frac{1}{2}\mathrm{Tr}\left(\sigma\sigma^{\mathrm{T}}(t,x)(\mathrm{Hess}_x u)(t,x)\right) + \nabla u(t,x)\cdot\mu(t,x)$$
$$+ f\left(t, x, u(t,x), \sigma^{\mathrm{T}}(t,x)\nabla u(t,x)\right) = 0 \qquad \textbf{[1]}$$

features:

label:

https://www.pnas.org/content/115/34/8505/tab-article-info

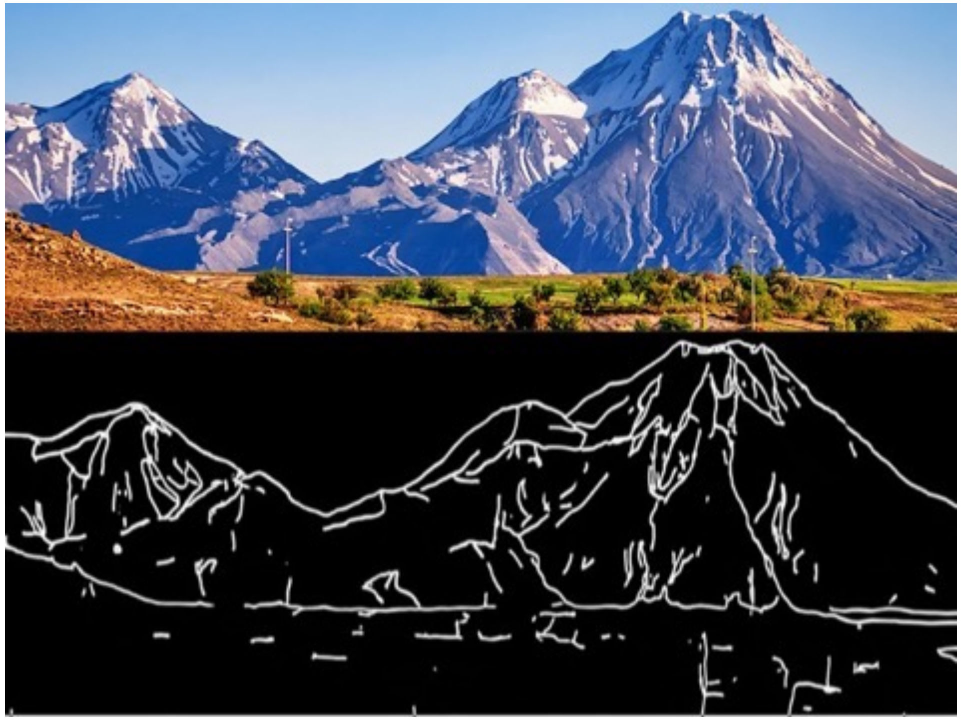
Datapoint = A Bridge

features:

label:

https://commons.wikimedia.org/wiki/Category:Bridges

Datapoint = Image Sketch



features:

label:

https://ml4a.net/

Datapoints, their Features and Labels are Design Choices!

raw data from FMI

https://en.ilmatieteenlaitos.fi/download-observations

Year	m	d	Time	precp	snow	airtmp	mintmp	maxtmp
2020	1	2	00:00	0,4	55	2,5	-2	4,5
2020	1	3	00:00	1,6	53	0,8	-0,8	4,6
2020	1	4	00:00	0,1	51	-5,8	-11,1	-0,7
2020	1	5	00:00	1,9	52	-13,5	-19,1	-4,6
2020	1	6	00:00	0,6	52	-2,4	-11,4	-1
2020	1	7	00:00	4,1	52	0,4	-2	1,3
2020	1	8	00:00	4,3	51	0,8	0,1	1,8
2020	1	9	00:00	-1	51	-0,6	-1,9	1,6
2020	1	10	00:00	-1	51	-6,2	-11	-1,4
2020	1	11	00:00	2,8	50	-4,8	-10,7	-2,1
2020	1	12	00:00	-1	53	-1,3	-3,5	0,9
2020	1	13	00:00	-1	53	-6,4	-12,9	-3,1
2020	1	14	00:00	9,7	52	-2,8	-9	-0,7
2020	1	15	00:00	-1	63	0,2	-0,7	0,6
2020	1	16	00:00	0,4	62	-3,9	-5,2	0,1
2020	1	17	00:00	2	62	-5,2	-8,4	-0,7

features

Year	m	d	Time	precp	snow	airtmp	mintmp	maxtmp
2020	1	2	00:00	0,4	55	2,5	-2	4,5
2020	1	3	00:00	1,6	53	0,8	-0,8	4,6
2020	1	4	00:00	0,1	51	-5,8	-11,1	-0,7
2020	1	5	00:00	1,9	52	-13,5	-19,1	-4,6
2020	1	6	00:00	0,6	52	-2,4	-11,4	-1
2020	1	7	00:00	4,1	52	0,4	-2	1,3
2020	1	8	00:00	4,3	51	0,8	0,1	1,8
2020	1	9	00:00	-1	51	-0,6	-1,9	1,6
2020	1	10	00:00	-1	51	-6,2	-11	-1,4
2020	1	11	00:00	2,8	50	-4,8	-10,7	-2,1
2020	1	12	00:00	-1	53	-1,3	-3,5	0,9
2020	1	13	00:00	-1	53	-6,4	-12,9	-3,1
2020	1	14	00:00	9,7	52	-2,8	-9	-0,7
2020	1	15	00:00	-1	63	0,2	-0,7	0,6
2020	1	16	00:00	0,4	62	-3,9	-5,2	0,1
2020	1	17	00:00	2	62	-5,2	-8,4	-0,7

label

data point

data point, features and label
are design choices!

```
newdataset= somedata[somedata['date'] == '2021-06-01'] ;
print(newdataset)
```

```
          date   time  temperature
0   2021-06-01  00:00          6.2
1   2021-06-01  01:00          6.4
2   2021-06-01  02:00          6.4
3   2021-06-01  03:00          6.8
4   2021-06-01  04:00          7.1
5   2021-06-01  05:00          7.6
6   2021-06-01  06:00          7.5
7   2021-06-01  07:00          8.1
8   2021-06-01  08:00         10.3
9   2021-06-01  09:00         12.8
10  2021-06-01  10:00         15.0
11  2021-06-01  11:00         14.1
12  2021-06-01  12:00         16.5
13  2021-06-01  13:00         13.6
14  2021-06-01  14:00         14.2
15  2021-06-01  15:00         13.3
16  2021-06-01  16:00         14.5
17  2021-06-01  17:00         13.8
```

Key Parameters of a Data Set

number n of features

number m of data points "sample size"

Year	m	d	Time	precp	snow	airtmp	mintmp	maxtmp
2020	1	2	00:00	0,4	55	2,5	-2	4,5
2020	1	3	00:00	1,6	53	0,8	-0,8	4,6
2020	1	4	00:00	0,1	51	-5,8	-11,1	-0,7
2020	1	5	00:00	1,9	52	-13,5	-19,1	-4,6
2020	1	6	00:00	0,6	52	-2,4	-11,4	-1
2020	1	7	00:00	4,1	52	0,4	-2	1,3
2020	1	8	00:00	4,3	51	0,8	0,1	1,8
2020	1	9	00:00	-1	51	-0,6	-1,9	1,6
2020	1	10	00:00	-1	51	-6,2	-11	-1,4
2020	1	11	00:00	2,8	50	-4,8	-10,7	-2,1
2020	1	12	00:00	-1	53	-1,3	-3,5	0,9
2020	1	13	00:00	-1	53	-6,4	-12,9	-3,1
2020	1	14	00:00	9,7	52	-2,8	-9	-0,7
2020	1	15	00:00	-1	63	0,2	-0,7	0,6
2020	1	16	00:00	0,4	62	-3,9	-5,2	0,1
2020	1	17	00:00	2	62	-5,2	-8,4	-0,7
2020	1	18	00:00	19,6	65	-4,6	-7,3	-4,2
2020	1	19	00:00	0,7	81	-4,4	-8,8	-2,7
2020	1	20	00:00	2,8	79	-1,8	-10,5	[illegible]

Feature Deluge.

modern information technology provides huge number of raw features

- smartphones
- webcams
- social networks
- smart watch
- ….

use only most relevant features but not fewer.

missing relevant features bad for accuracy

using many irrelevant features wastes computation and might result in overfitting

```
newdataset= somedata[somedata['date'] == '2021-06-01'] ;
print(newdataset)
```

```
          date   time  temperature
0   2021-06-01  00:00          6.2
1   2021-06-01  01:00          6.4
2   2021-06-01  02:00          6.4
3   2021-06-01  03:00          6.8
4   2021-06-01  04:00          7.1
5   2021-06-01  05:00          7.6
6   2021-06-01  06:00          7.5
7   2021-06-01  07:00          8.1
8   2021-06-01  08:00         10.3
9   2021-06-01  09:00         12.8
10  2021-06-01  10:00         15.0
11  2021-06-01  11:00         14.1
12  2021-06-01  12:00         16.5
13  2021-06-01  13:00         13.6
14  2021-06-01  14:00         14.2
15  2021-06-01  15:00         13.3
16  2021-06-01  16:00         14.5
17  2021-06-01  17:00         13.8
```

data point = some day at FMI station

feature = nr of hourly observations

want to predict maximum daytime temperature

missing relevant features bad for accuracy

```
newdataset= somedata[somedata['date'] == '2021-06-01'] ;
print(newdataset)
```

```
          date   time  temperature
0   2021-06-01  00:00          6.2
1   2021-06-01  01:00          6.4
2   2021-06-01  02:00          6.4
3   2021-06-01  03:00          6.8
4   2021-06-01  04:00          7.1
5   2021-06-01  05:00          7.6
6   2021-06-01  06:00          7.5
7   2021-06-01  07:00          8.1
8   2021-06-01  08:00         10.3
9   2021-06-01  09:00         12.8
10  2021-06-01  10:00         15.0
11  2021-06-01  11:00         14.1
12  2021-06-01  12:00         16.5
13  2021-06-01  13:00         13.6
14  2021-06-01  14:00         14.2
15  2021-06-01  15:00         13.3
16  2021-06-01  16:00         14.5
17  2021-06-01  17:00         13.8
```

data point = some day at FMI station

feature = hourly temp. 00:00 – 15:00

want to predict temp at 16:00

using irrelevant features wastes comp. resources

Label is Design Choice!

YOU choose the label of a data point

by choosing/defining label you define the ML problem or learning task !

Lecture continues at 15:30

Regression. Numeric Labels.

	date	time	temperature
0	2021-06-01	00:00	6.2
1	2021-06-01	01:00	6.4
2	2021-06-01	02:00	6.4
3	2021-06-01	03:00	6.8
4	2021-06-01	04:00	7.1
5	2021-06-01	05:00	7.6
6	2021-06-01	06:00	7.5
7	2021-06-01	07:00	8.1
8	2021-06-01	08:00	10.3
9	2021-06-01	09:00	12.8
10	2021-06-01	10:00	15.0
11	2021-06-01	11:00	14.1
12	2021-06-01	12:00	16.5
13	2021-06-01	13:00	13.6
14	2021-06-01	14:00	14.2
15	2021-06-01	15:00	13.3
16	2021-06-01	16:00	14.5
17	2021-06-01	17:00	13.8

datapoint
“2021-06-01 at some FMI station”

label = tmp at 15:00

Binary Classification.

	date	time	temperature
0	2021-06-01	00:00	6.2
1	2021-06-01	01:00	6.4
2	2021-06-01	02:00	6.4
3	2021-06-01	03:00	6.8
4	2021-06-01	04:00	7.1
5	2021-06-01	05:00	7.6
6	2021-06-01	06:00	7.5
7	2021-06-01	07:00	8.1
8	2021-06-01	08:00	10.3
9	2021-06-01	09:00	12.8
10	2021-06-01	10:00	15.0
11	2021-06-01	11:00	14.1
12	2021-06-01	12:00	16.5
13	2021-06-01	13:00	13.6
14	2021-06-01	14:00	14.2
15	2021-06-01	15:00	13.3
16	2021-06-01	16:00	14.5
17	2021-06-01	17:00	13.8

datapoint
"2021-06-01 at some FMI station"

label =

- "hot" if tmp at 15:00 > 10
- "cold" if … <= 10

Multi-Class Classification

	date	time	temperature
0	2021-06-01	00:00	6.2
1	2021-06-01	01:00	6.4
2	2021-06-01	02:00	6.4
3	2021-06-01	03:00	6.8
4	2021-06-01	04:00	7.1
5	2021-06-01	05:00	7.6
6	2021-06-01	06:00	7.5
7	2021-06-01	07:00	8.1
8	2021-06-01	08:00	10.3
9	2021-06-01	09:00	12.8
10	2021-06-01	10:00	15.0
11	2021-06-01	11:00	14.1
12	2021-06-01	12:00	16.5
13	2021-06-01	13:00	13.6
14	2021-06-01	14:00	14.2
15	2021-06-01	15:00	13.3
16	2021-06-01	16:00	14.5
17	2021-06-01	17:00	13.8

datapoint
"2021-06-01 at some FMI station"

label =

- "nice morning" if tmp at 15:00 < 10 and tmp at 10:00 > 10
- "nice noon" if tmp at 15:00 > 10 and tmp at 10:00 < 10
- "nice day" if tmp at 15:00 > 10 and tmp at 10:00 > 10

Multilabel Problems – Multitask Learning

by choosing/defining label you define the ML task !

for same data, use different labels → multiple learning tasks

multi-label class. (special case of multi-task learning)

Multi-Label Regression.

	date	time	temperature
0	2021-06-01	00:00	6.2
1	2021-06-01	01:00	6.4
2	2021-06-01	02:00	6.4
3	2021-06-01	03:00	6.8
4	2021-06-01	04:00	7.1
5	2021-06-01	05:00	7.6
6	2021-06-01	06:00	7.5
7	2021-06-01	07:00	8.1
8	2021-06-01	08:00	10.3
9	2021-06-01	09:00	12.8
10	2021-06-01	10:00	15.0
11	2021-06-01	11:00	14.1
12	2021-06-01	12:00	16.5
13	2021-06-01	13:00	13.6
14	2021-06-01	14:00	14.2
15	2021-06-01	15:00	13.3
16	2021-06-01	16:00	14.5
17	2021-06-01	17:00	13.8

datapoint
"2021-06-01 at some FMI station"

label1 = tmp at 10:00

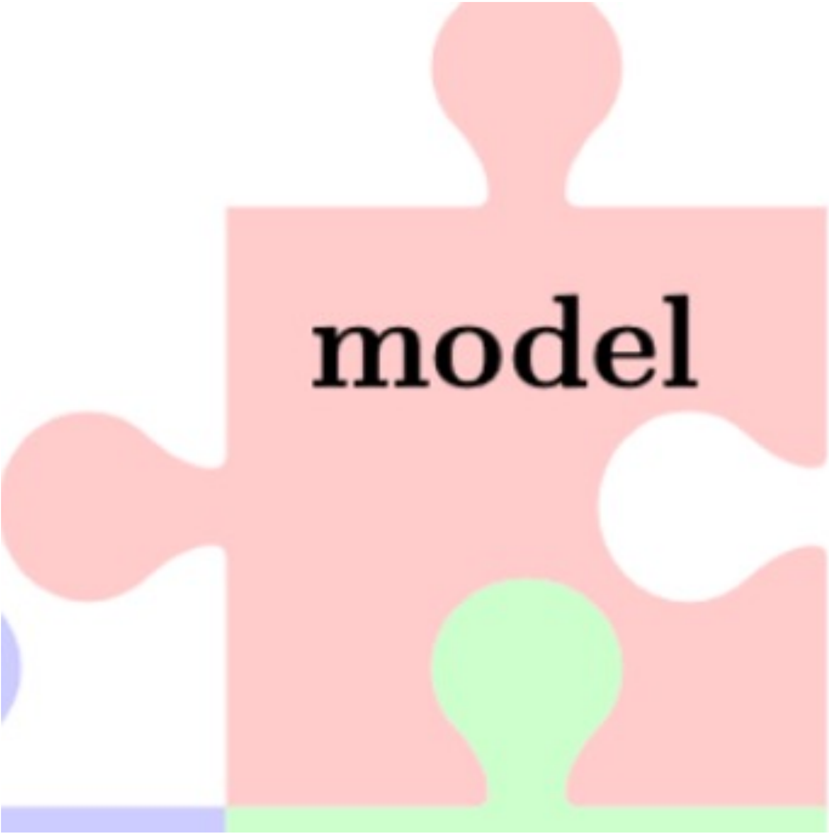
label2= tmp at 15:00

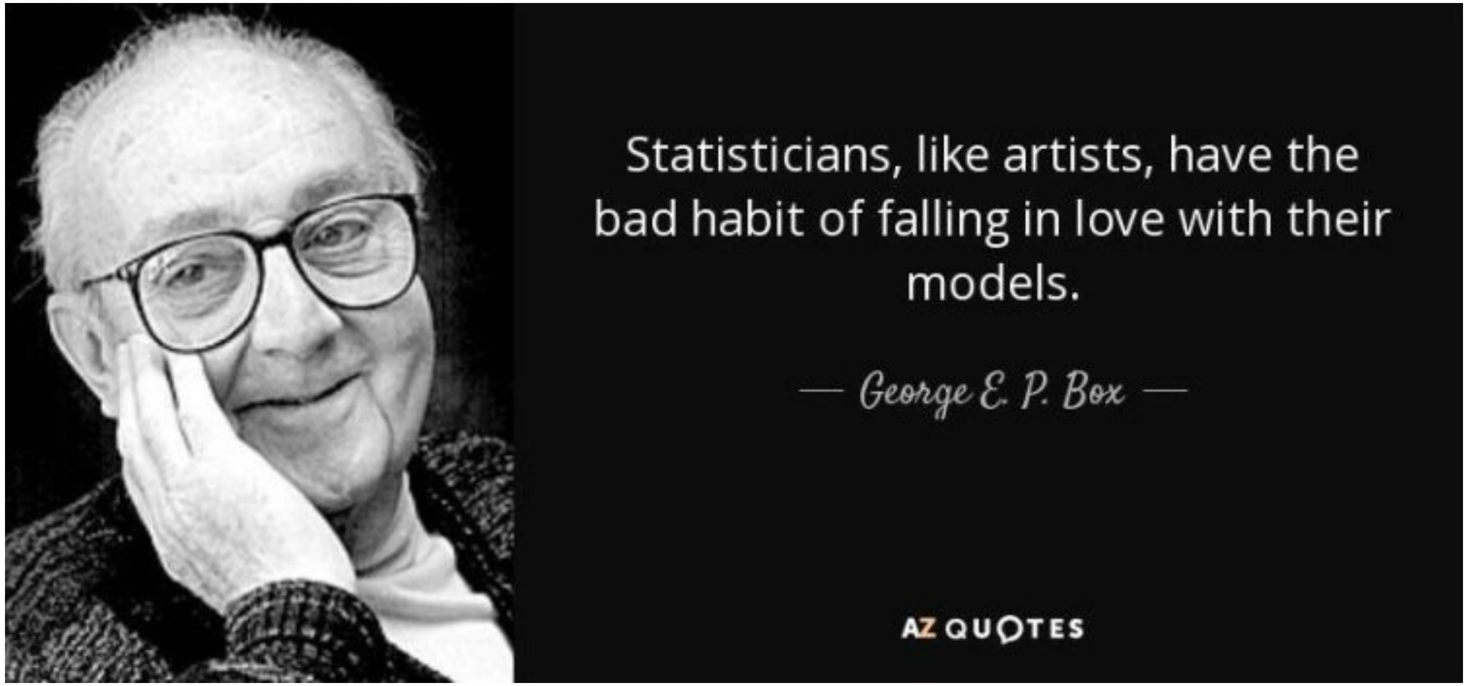
Multilabel Classification.

y_1= 1 or 0 if car present or not

y_2= 1 or 0 if person present or not

y_3= 1 or 0 if tree present or not

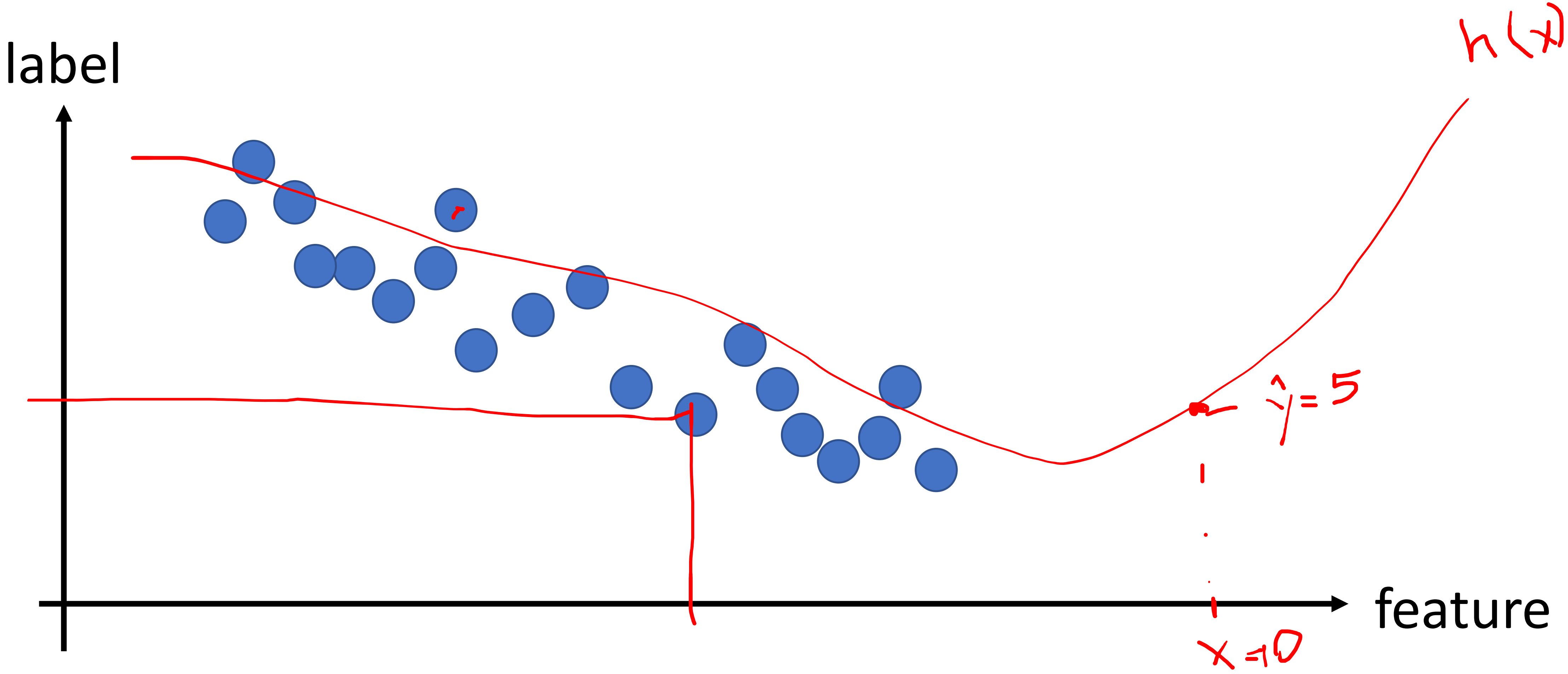

model


Statisticians, like artists, have the bad habit of falling in love with their models.
— George E. P. Box —
AZ QUOTES

Machine Learning.

"learn to predict the label of a data point solely from its features"

Scatterplot

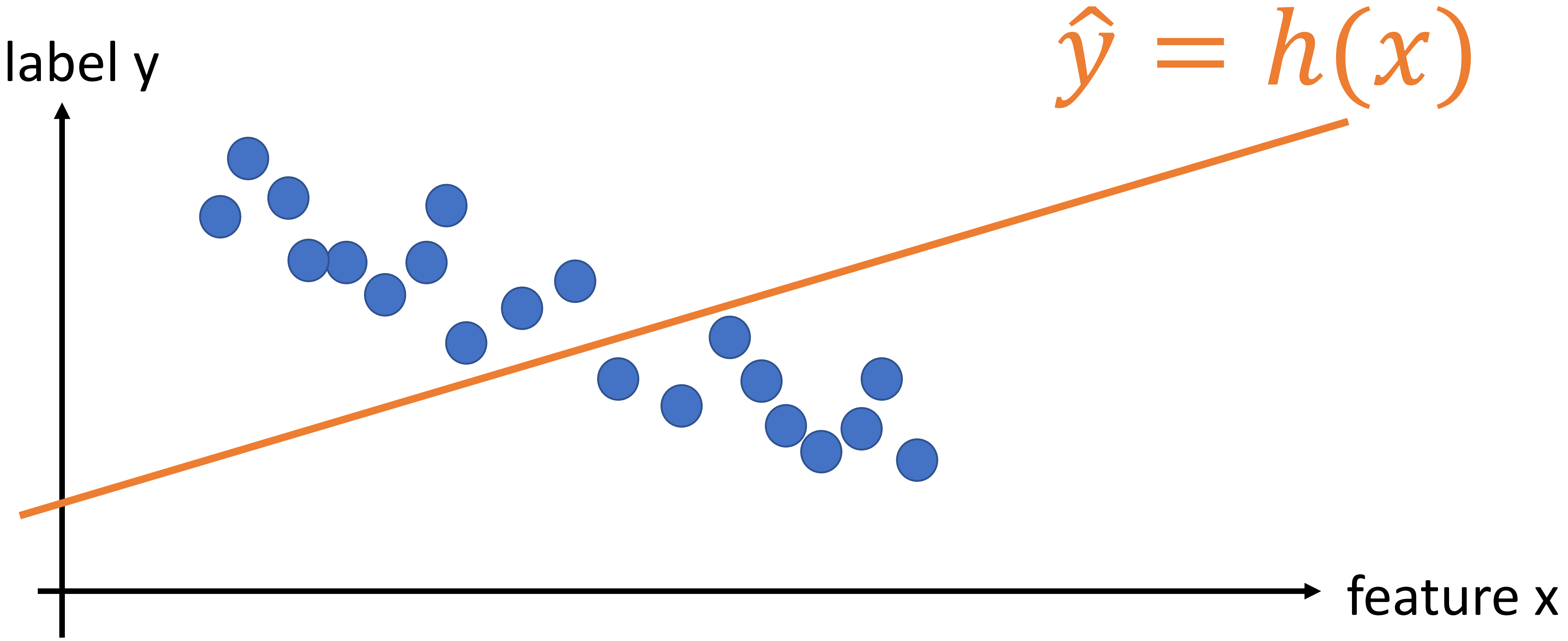


How to Predict?

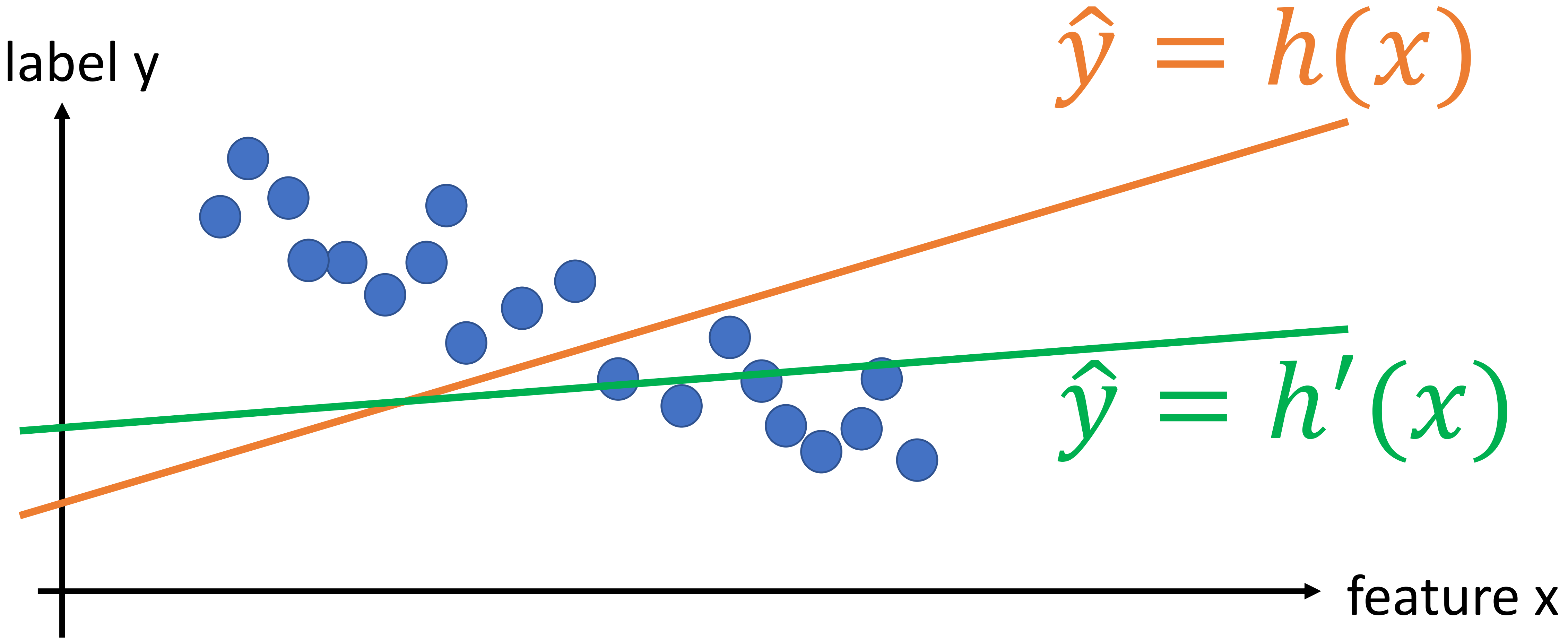
apply a hypothesis map h to features x,

$$\hat{y} = h(x)$$

A Hypothesis.



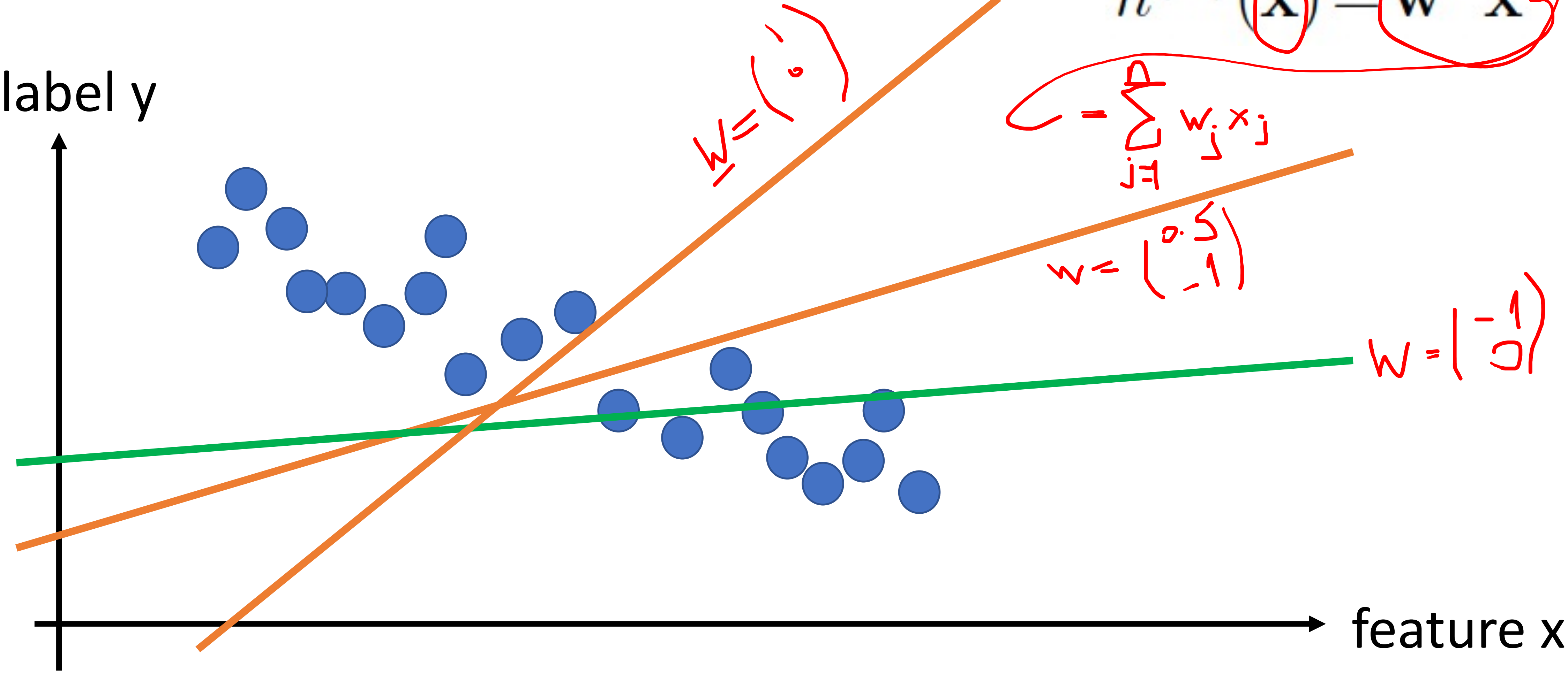
Model = Several Hypotheses.



Linear Model

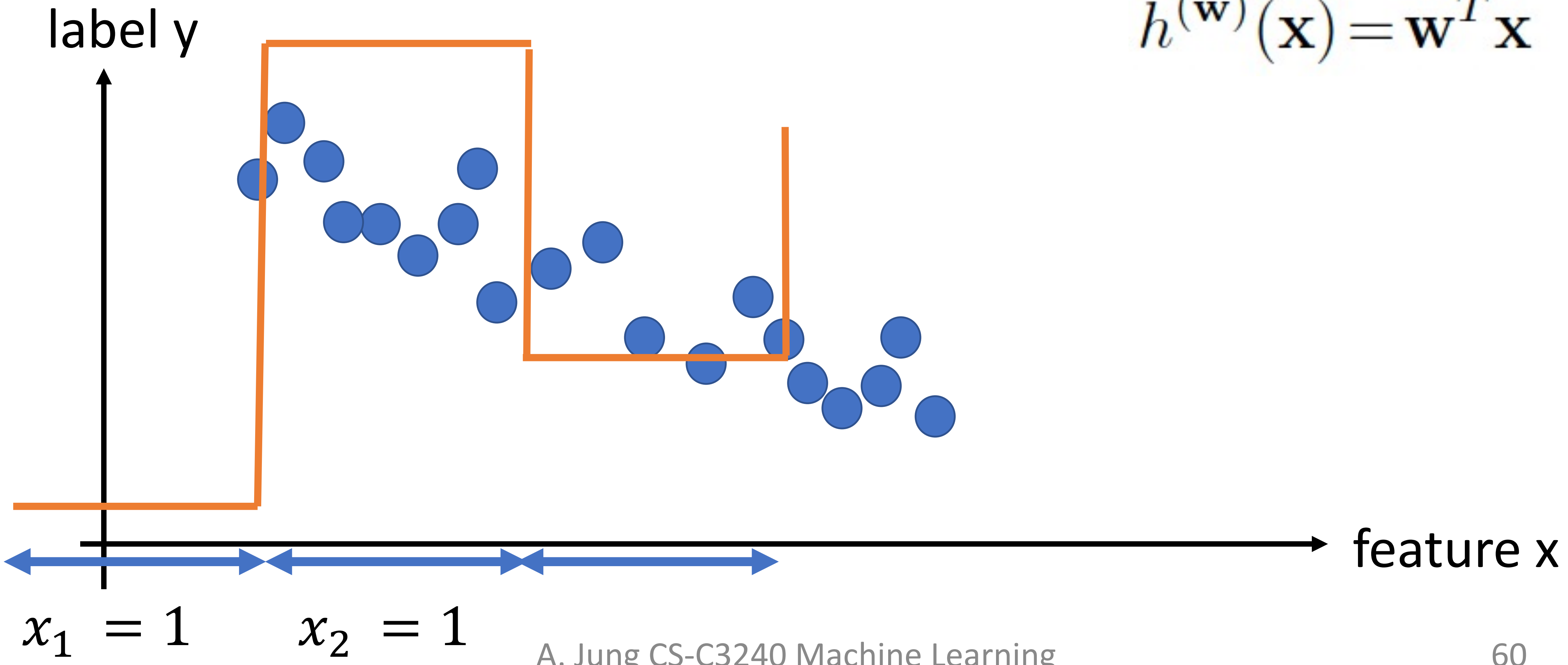
$$h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_{j=1}^{n} w_j x_j$$

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



Linear Model is Versatile!

$$h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$



Linear + Feature Map

feature map

$\phi(\cdot)$

single feature x

$$\begin{pmatrix} x_1 = \phi_1(x) \\ x_2 = \phi_2(x) \\ \vdots \\ x_n = \phi_n(x) \end{pmatrix}$$

linear map

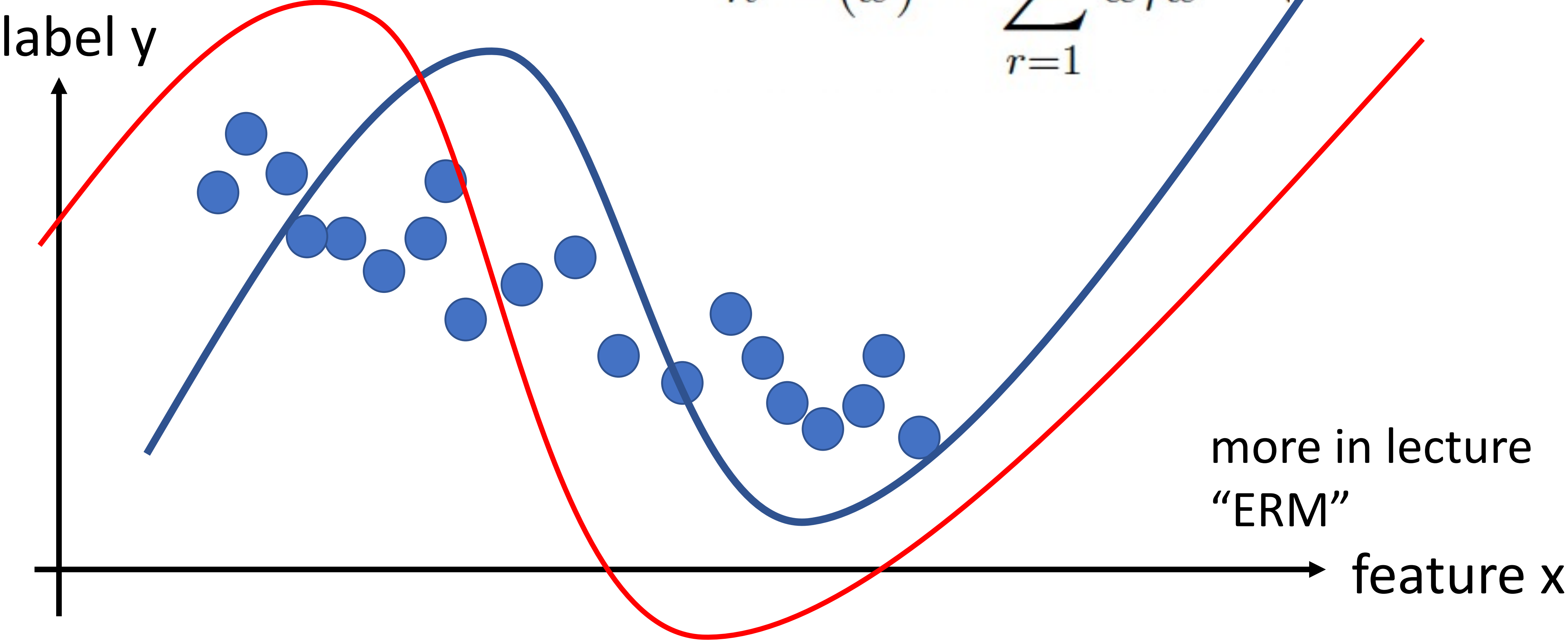
$$\mathbf{w}^T\mathbf{x} = \sum_{j=1}^{n} w_j x_j$$

h(x)

$$h(x) = \sum_{j=1}^{n} w_j \phi_j(x)$$

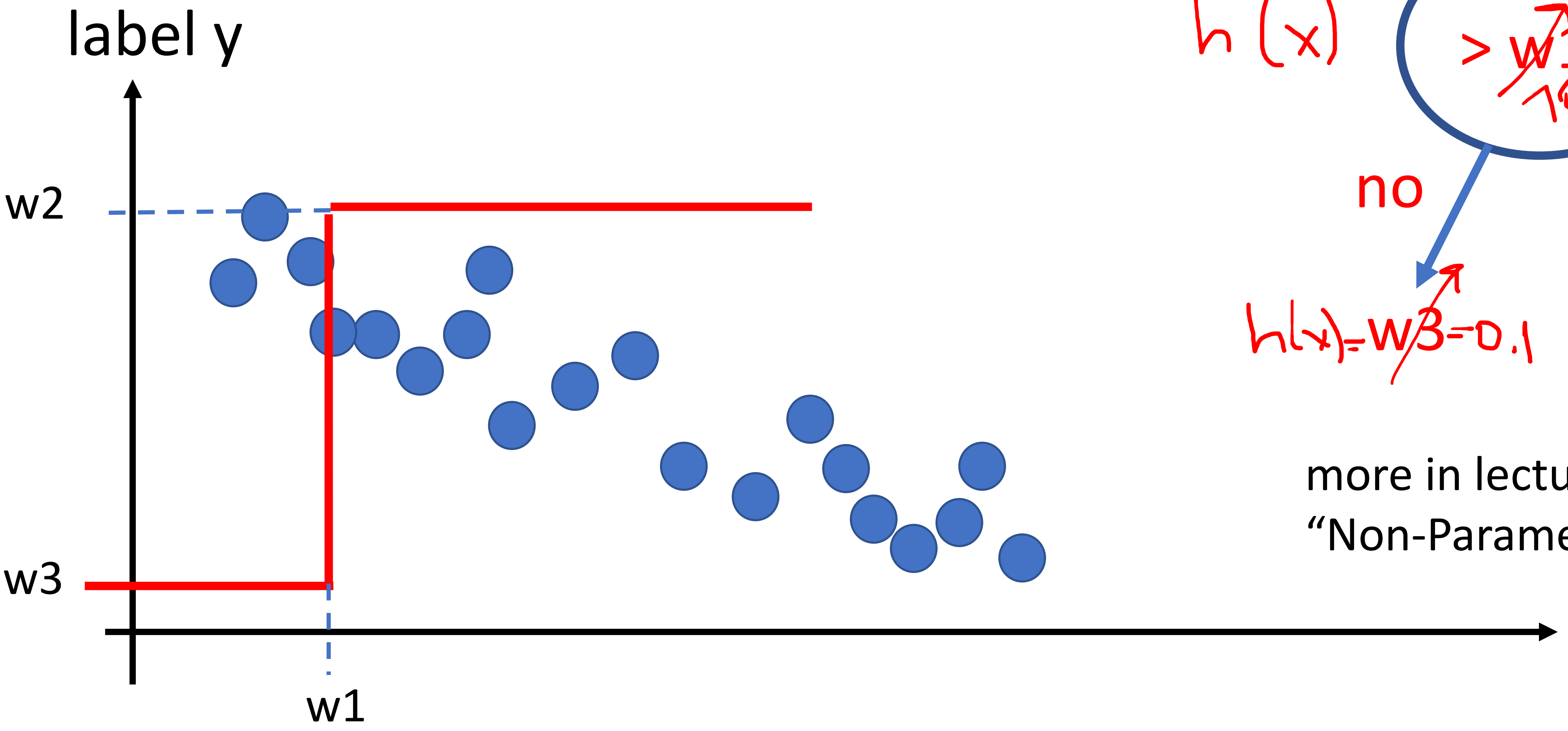
Polynomials

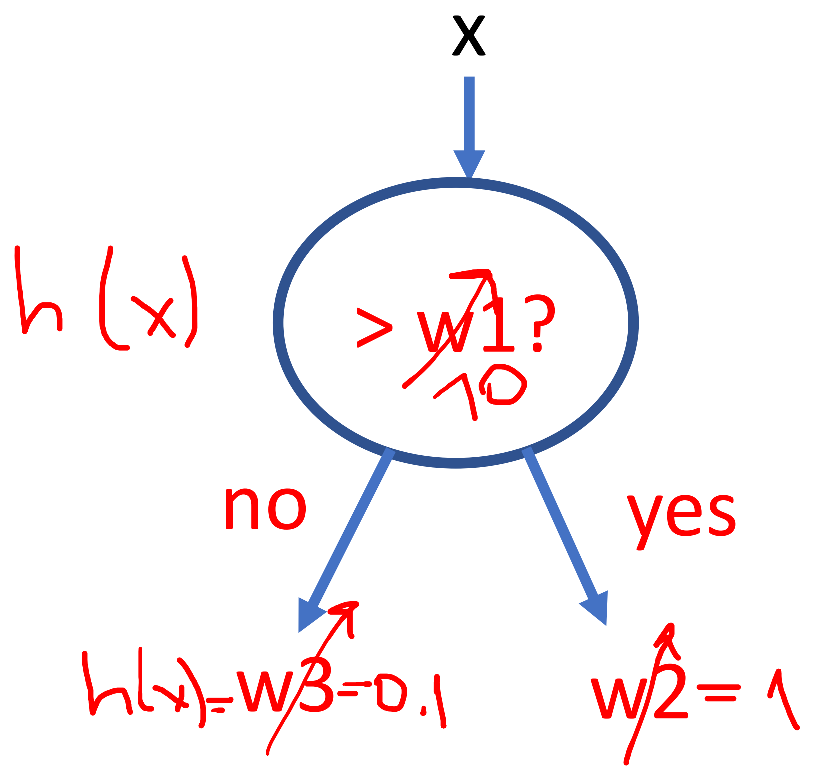
$$h^{(\mathbf{w})}(x) = \sum_{r=1}^{n} w_r x^{r-1}.$$



more in lecture "ERM"

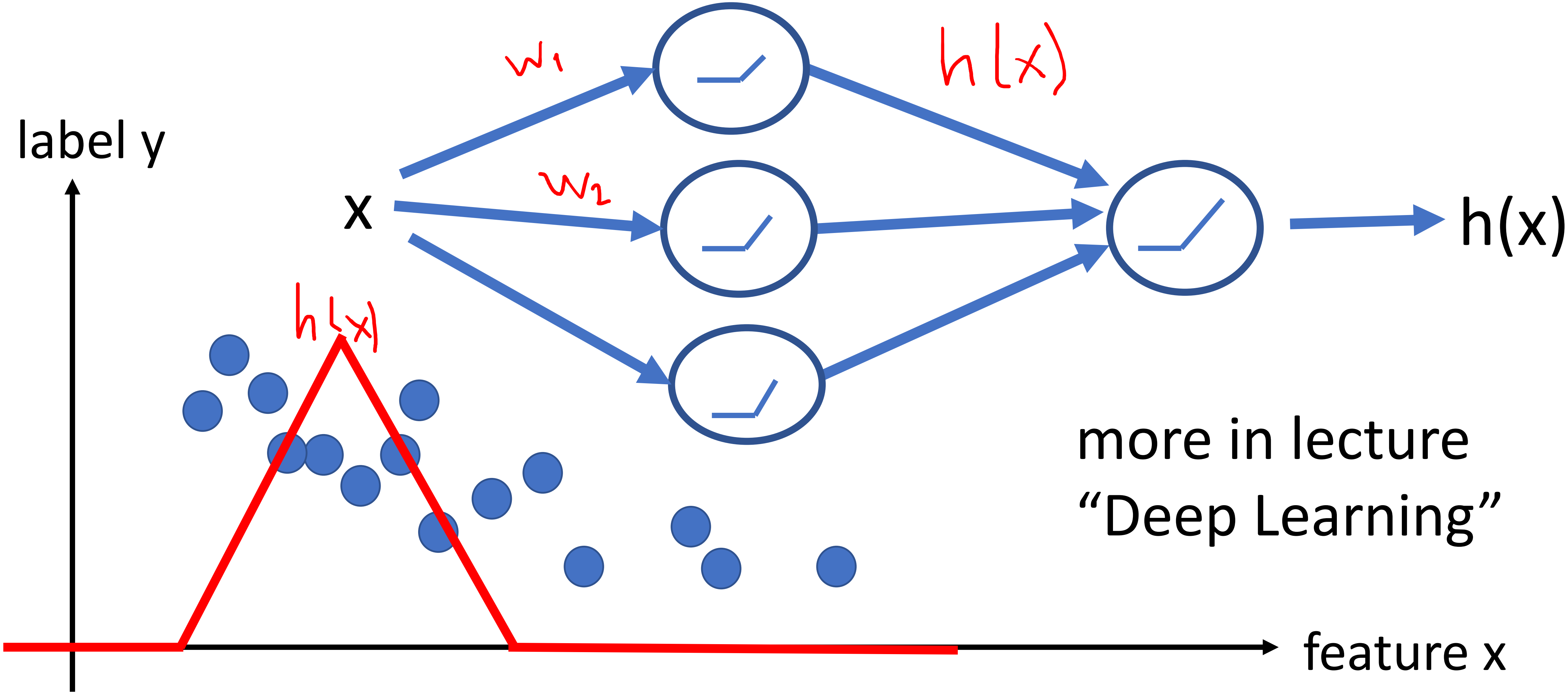
Decision Tree





more in lecture
"Non-Parametric Models"

Artificial Neural Network

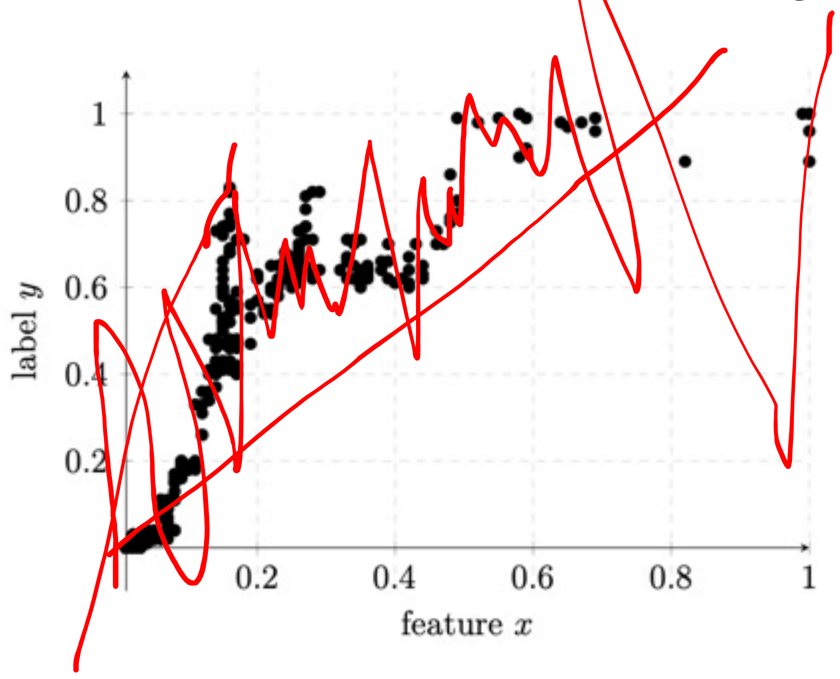


more in lecture
"Deep Learning"

Which Model To Choose?

- large to contain a good hypothesis
- small/simple to fit computational resources
- small to avoid overfitting

Sufficiently Large



linear model might be to small for such data

there is no straight line that fits well the data points here

need larger models that also contain non-linear maps

more on large (non-linear) models in Lectures "Deep Learning" and "Non-Parametric Models"

Sufficiently Small (Statistically)

- using too large model provokes overfitting
- model fits well training data but does a very poor job outside the training data

more on overfitting in Lectures
“Model Val/Sel” and “Diagnosing ML”

Sufficiently Small (Comput.)

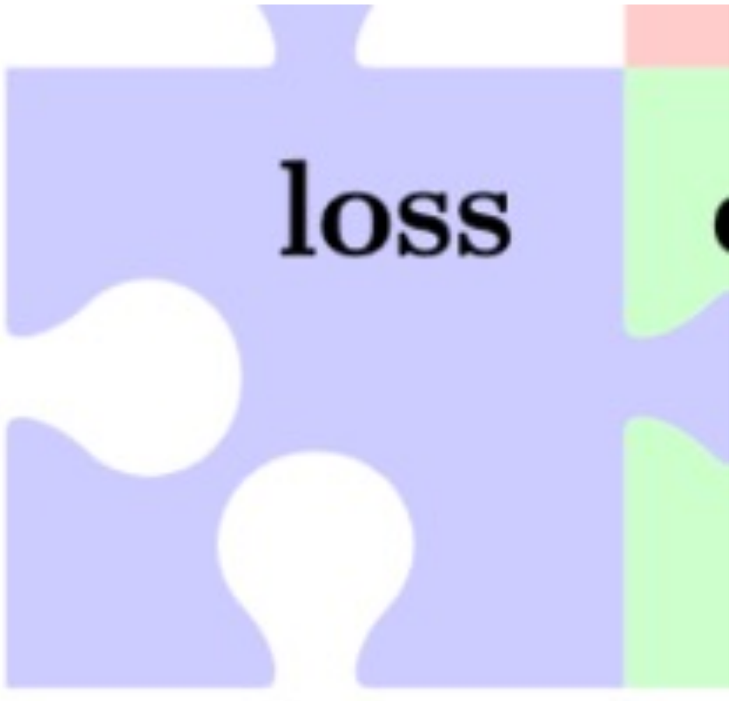
- consider linear model with n parameters

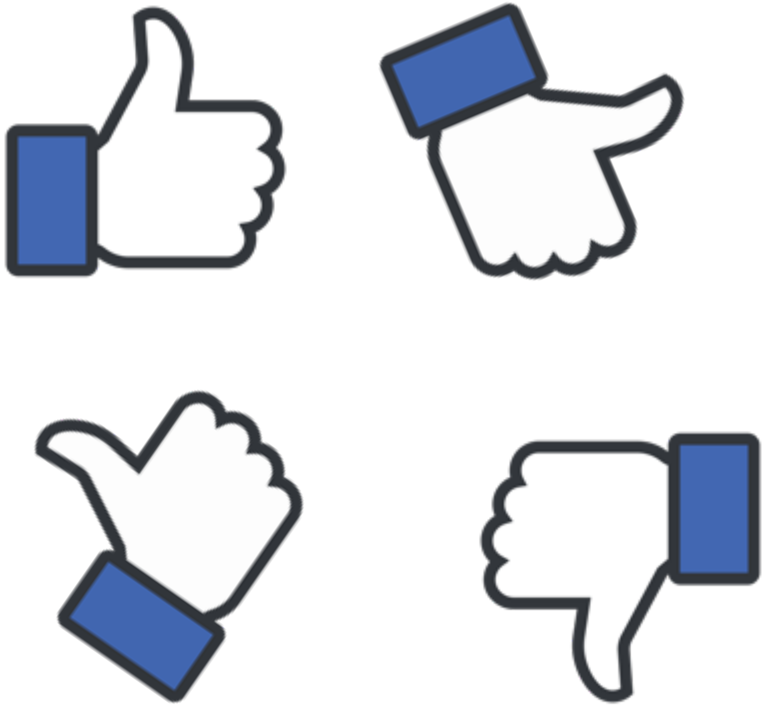
- fit linear model on m > n datapoints
- requires to invert a “n by n” matrix ! (see Secion 4.3 of http://mlbook.cs.aalto.fi)

Sufficiently Simple (Comput.)

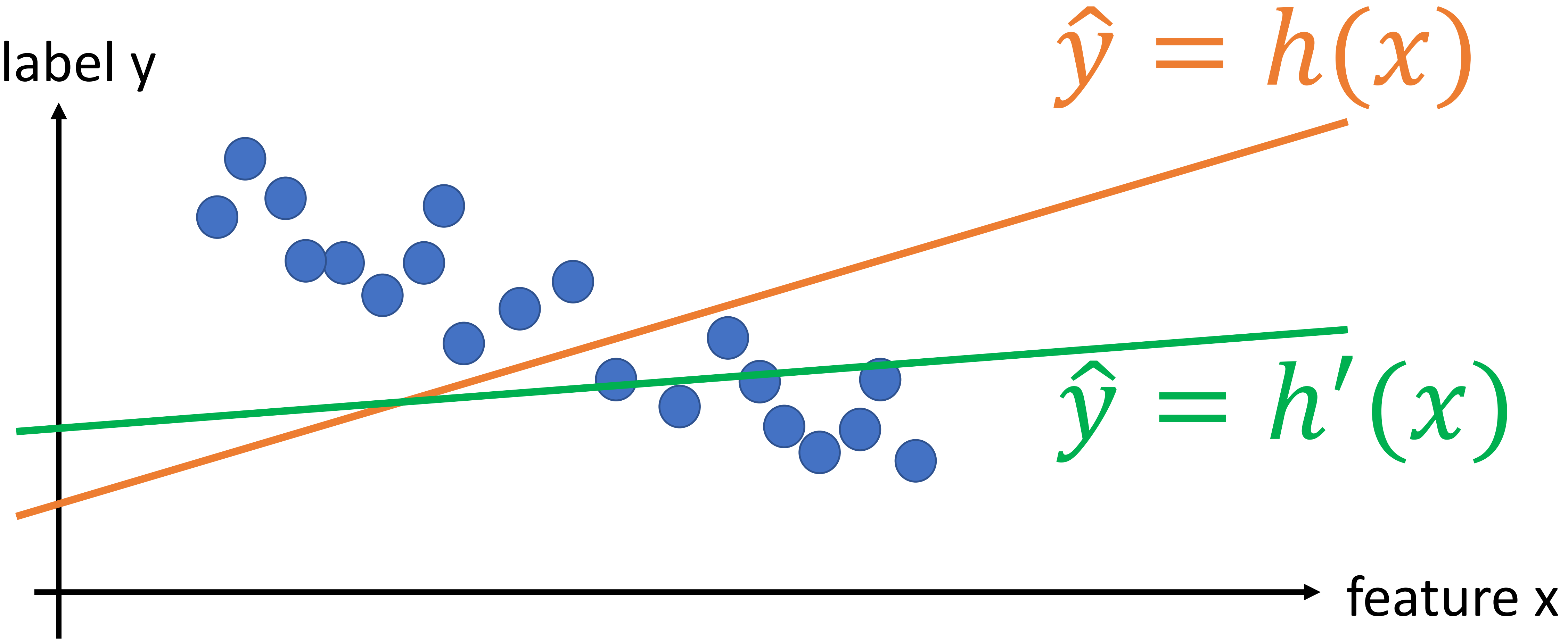
- hypothesis maps h(x) should be easy to evaluate
- recent MSc thesis on “Predicting Gas Valve Position”
- h(x) is used for engine control

compute h(x) in real-time (while engine is running!)

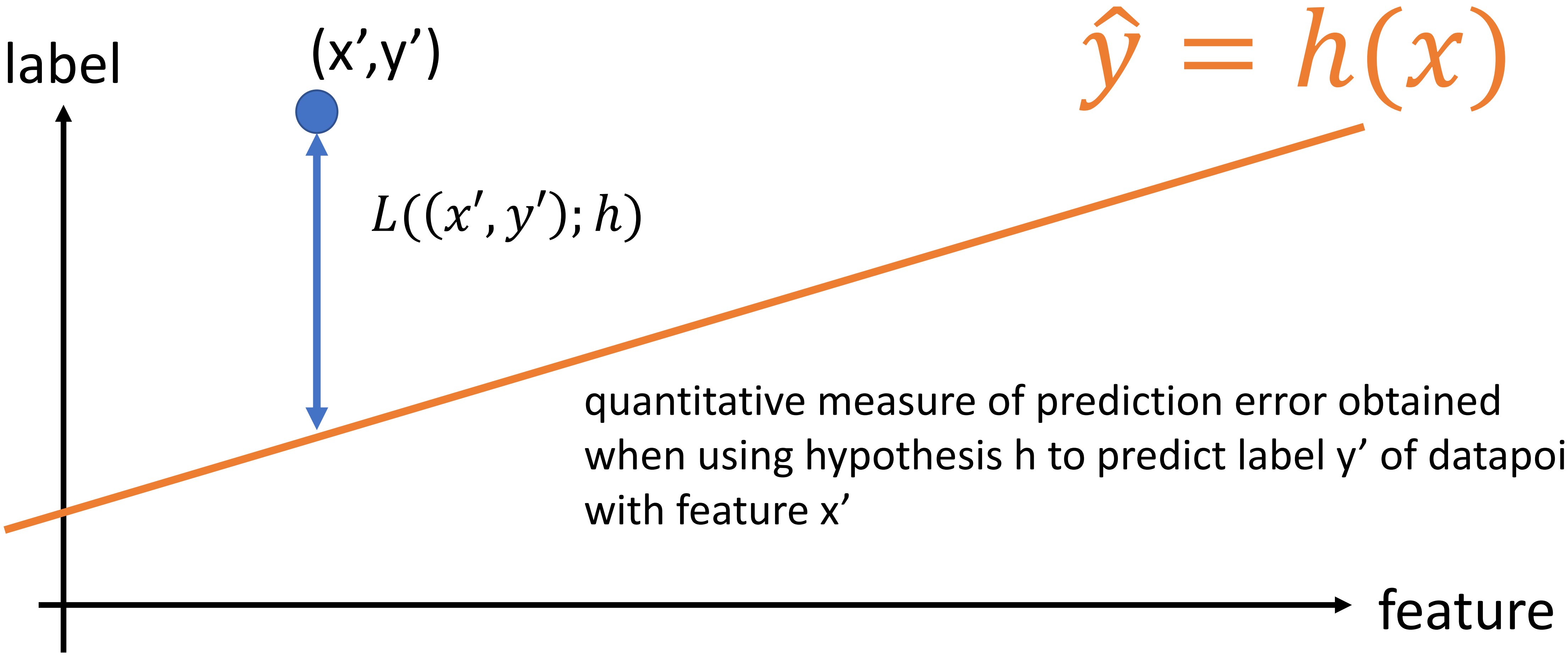

loss



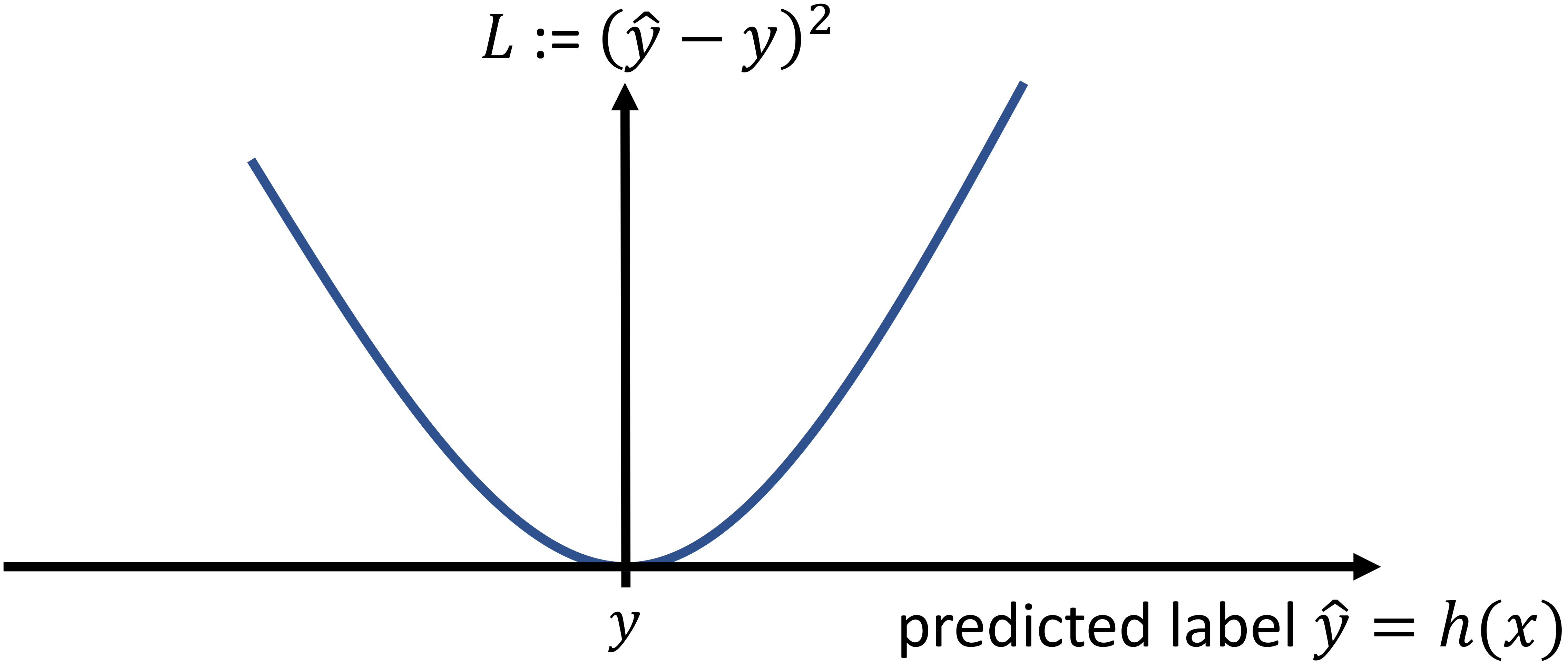
Which Hypothesis is Better?



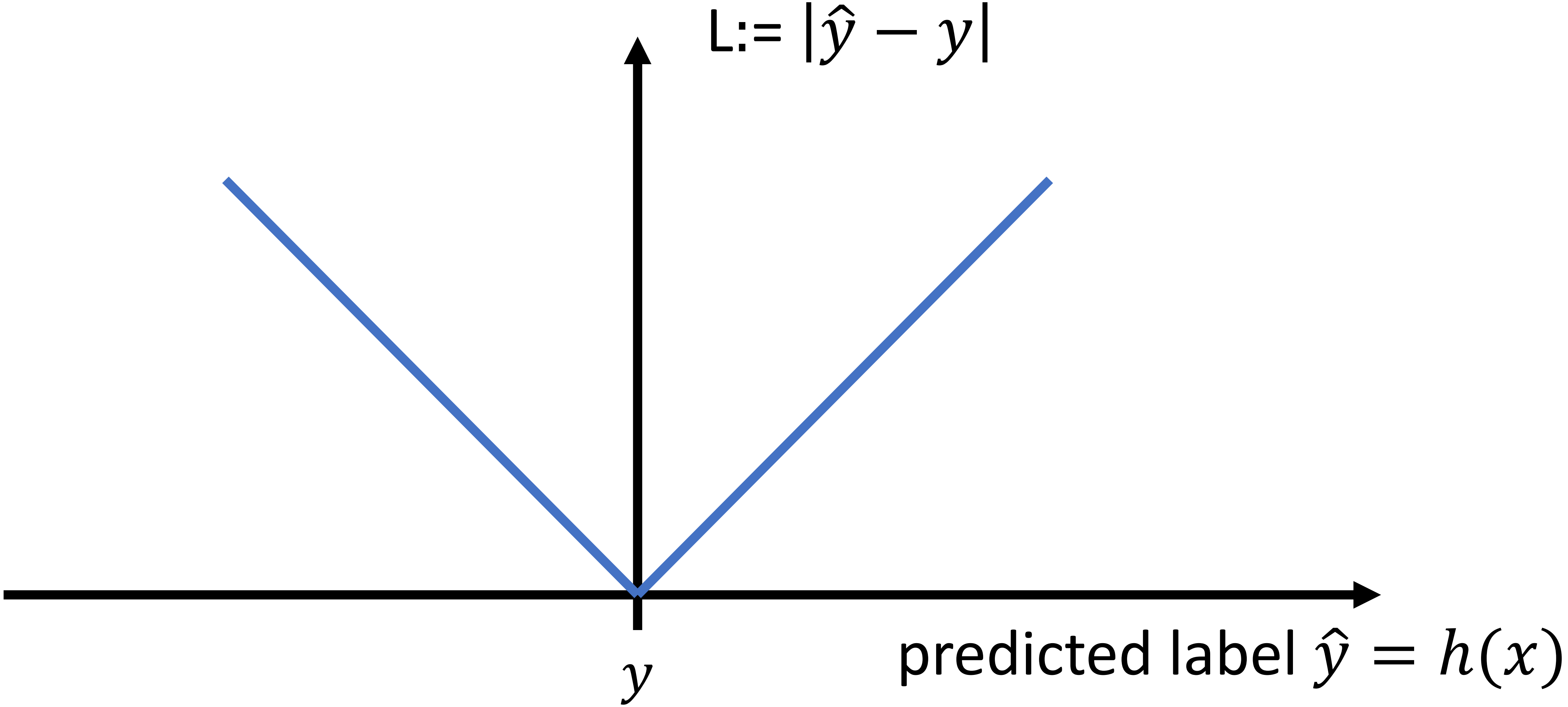
A Loss Function



The Squared Error Loss

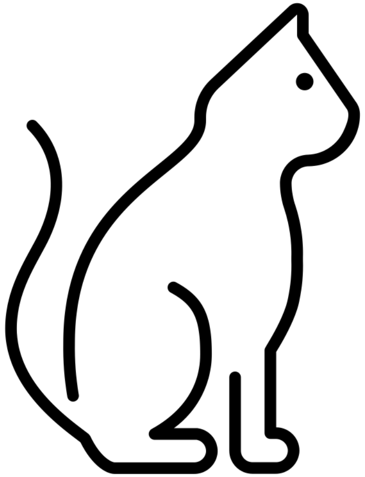


The Absolute Error Loss



Loss Functions for Binary Classification

label y = “cat”



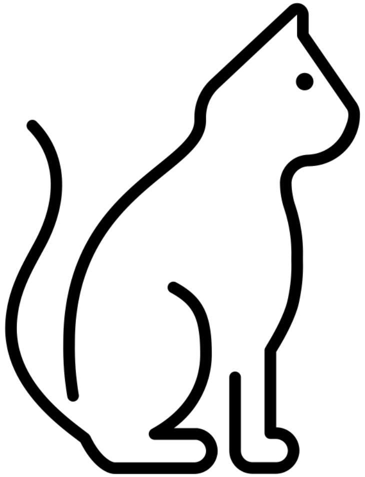
h(x) = “dog”

features x = pixels

Loss = 100

Loss Functions for Binary Classification

label y = “cat”



features x = pixels

h(x) = “cat”

Loss = 0

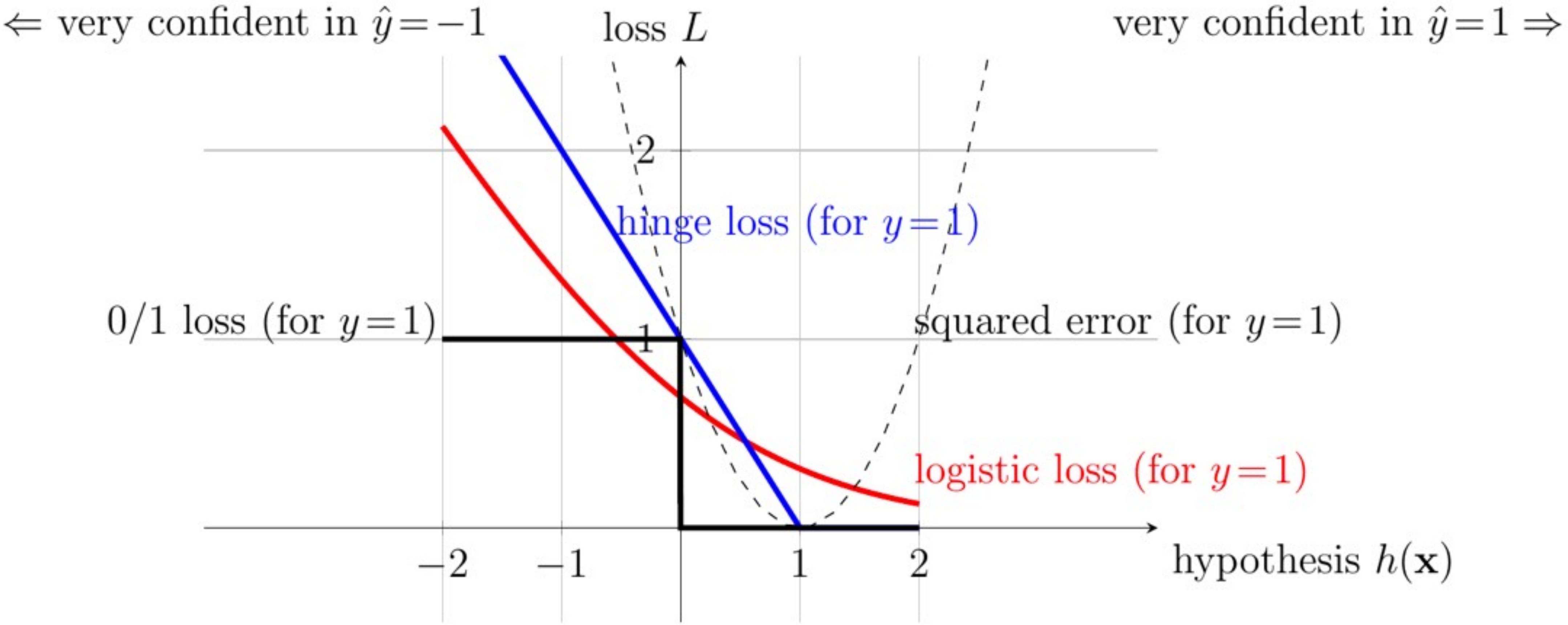
Classifiers

- consider label values either “cat” or “dog”

- features vector x = pixels values
- can we use linear hypothesis maps h(x)?

- YES!
- use sign h(x) to classify: h(x) > 0 → “dog”
- use |h(x)| as confidence measure

Loss Functions for Binary Classification



more on this in lecture "Classification"

Which Loss Function ?

- statistical aspects (should favour “reasonable” hypothesis)

- computational aspects (must be able to minimize them)

- interpretation (what does log-loss = -3 mean ?)

…..choosing a suitable loss function is often non-trivial !

Recent Paper about Coming up with a Good Loss Function

Algorithm 1 Generalized ground truth matching method for typical object detector performance evaluation.

Input:	$\mathcal{B}^p = \{(b_i^p, s_i)\}_{i=1}^D$	D bounding box predictions sorted by decreasing confidence score s_i for class c from input image $\mathbf{I}$.
	$\mathcal{B}^g = \{b_k^g\}_{k=1}^N$	N ground truth bounding box labels for class c from input image $\mathbf{I}$.
	$\varepsilon \in [0,1] \subset \mathbb{R}$	Box IoU threshold for matching.
	$g_{\max} \in \mathbb{N}$	Maximum number of GT boxes b_k^g to match with a single prediction b_i^p.
	$a_{\min} \in [0,1] \subset \mathbb{R}$	Minimum value for $A(b_k^p)/A(b_k^g)$, which limits TP prediction box size.
Output:	$\mathcal{Y} \in \{0,1\}^X$	A binary sequence of variable length $X \in \mathbb{N}_0$ indicating true and false positives, if $g_{\max} = 1 \Rightarrow X = D$.

function MATCHBOXESGENERIC($\mathcal{B}^p, \mathcal{B}^g, \varepsilon, g_{\max}, a_{\min}$)

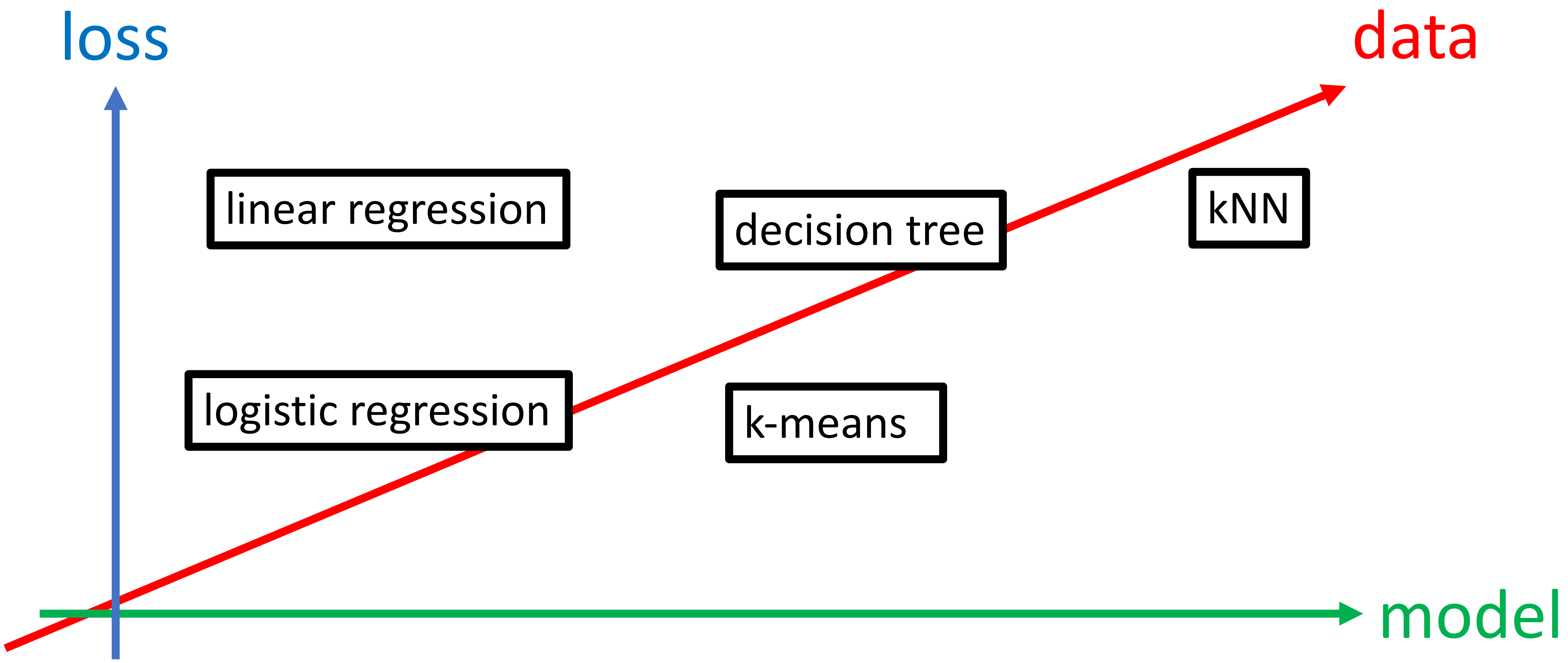
$\quad \mathcal{Y} \leftarrow \emptyset$

https://arxiv.org/pdf/2111.09406.pdf

Main Components of ML

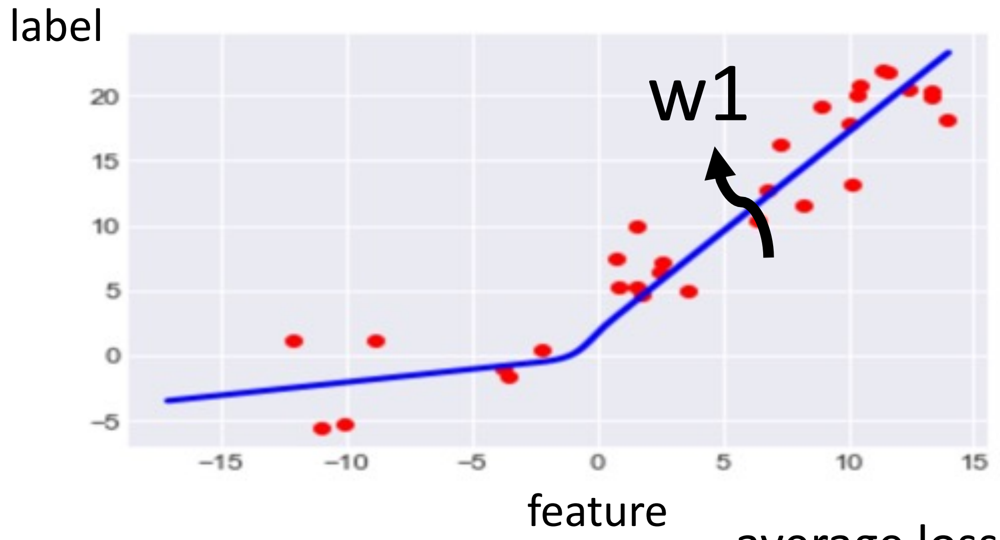
- data
- model
- loss

Landscape of ML Methods

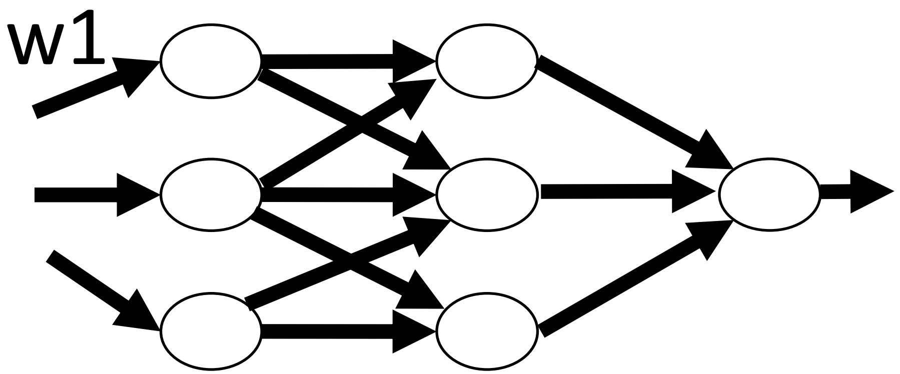


Three Views on Machine Learning

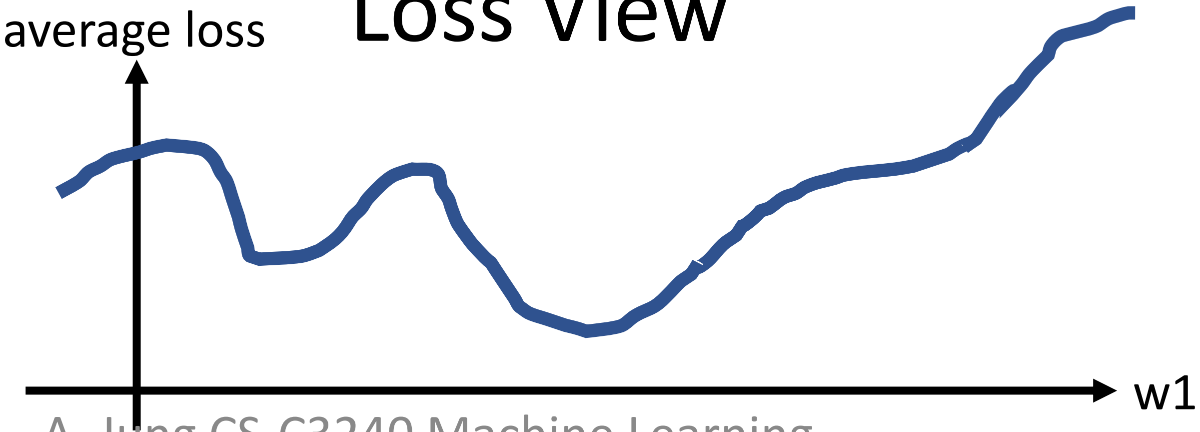
“Data View”



“Model View”



“Loss View”

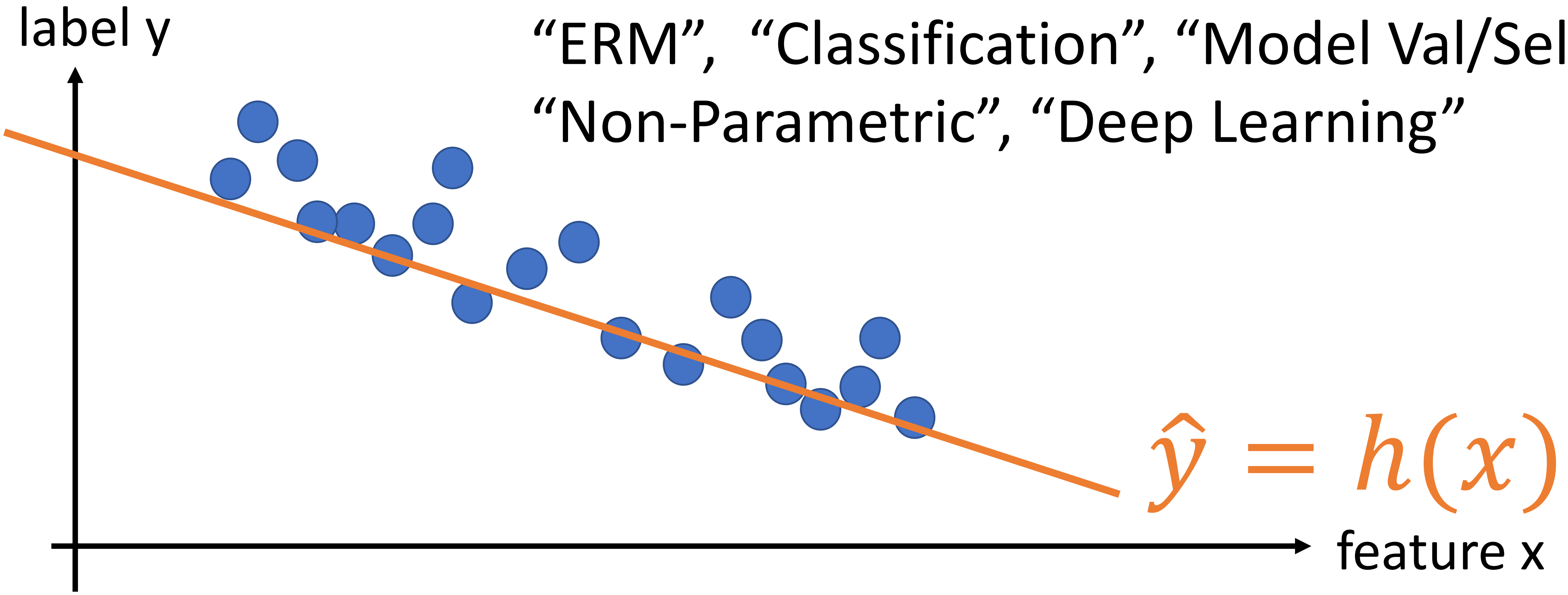


Three Main Flavours of ML

- supervised ML (use labeled data to imitate teacher)
- unsupervised ML (no labeled data needed)
- reinforcement learning (learn while collecting data)

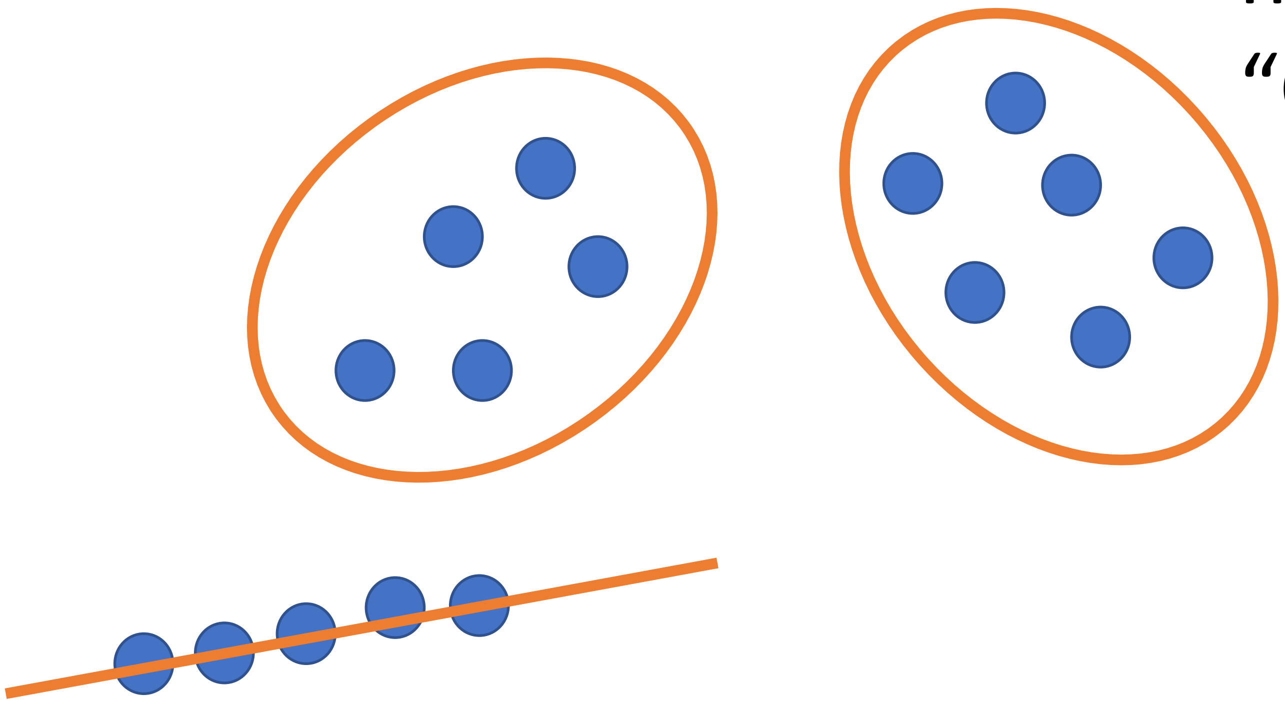
Supervised Learning

more on this in lecture:
"ERM", "Classification", "Model Val/Sel", "Non-Parametric", "Deep Learning"



Unsupervised Learning

more on this in Lecture “Clustering”, “Feature Learning”



label of datapoint = cluster assignment or nearby subspace

Reinforcement Learning

label = “optimal steering direction”

more on this in ELEC-E8125 - Reinforcement learning.

Wrap Up

- data points characterized by features and label
- features ≈ low-level properties
- labels ≈ high-level properties (quantity of interest)
- GOAL of ML: learn a hypothesis h such that h(x) $\approx y$
- ML model = comp. tractable subset of possible hypothesis maps h(x)
- prediction error y-h(x) quantified using a loss function

Next Lecture Wed. 16:15 "Empirical Risk Minimization"

GOAL of ML: Learn hypothesis h(.) such that y $\approx$ h(x) for any data point (x,y).

what exactly is "any data point" ?