Three Components of Deep Learning

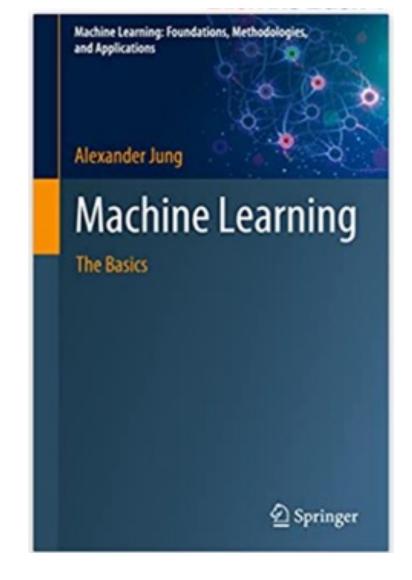
Alex(ander) Jung Assistant Professor for Machine Learning Department of Computer Science Aalto University

Learning Goals

- develop intuition for how ML works
- become familiar with concept of
 - data points (features, labels)
 - model (hypothesis space)
 - loss function (quality measure)

Reading.

Chapter 1,2 of [MLBook]





https://numpy.org/doc/stable/user/absolute_beginners.html

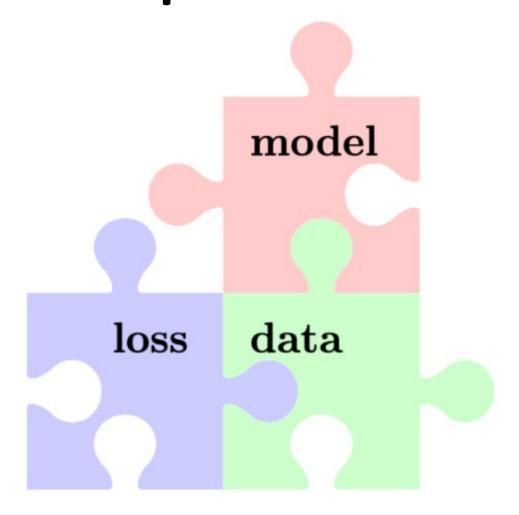
What is it all About?

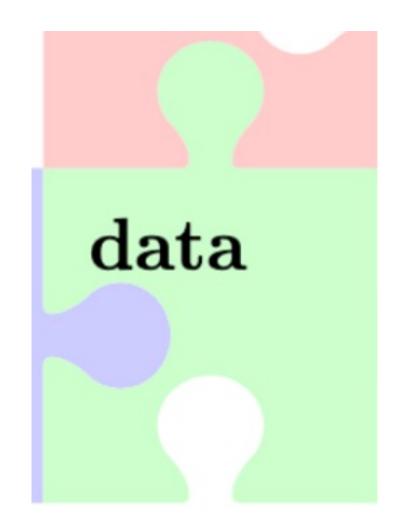
fit model to data to make accurate

predictions or forecasts!

"data" 4, 5, 6, 7, 8, "model" "hypothesis"

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

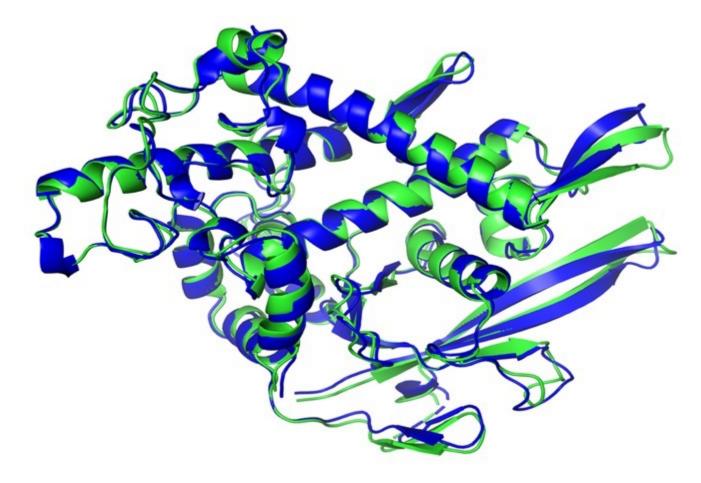
https://read.deeplearning.ai/the-batch/issue-84/

data = set of datapoints

What is a Datapoint?

some object that carries relevant information

Datapoint = Some Protein



Datapoint = A Partial Differential Equation

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

RESEARCH ARTICLE



Solving high-dimensional partial differential equations using deep learning

D Jiegun 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 = Some Cow



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.

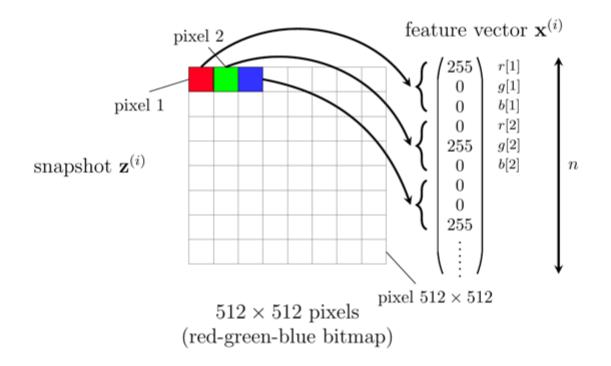
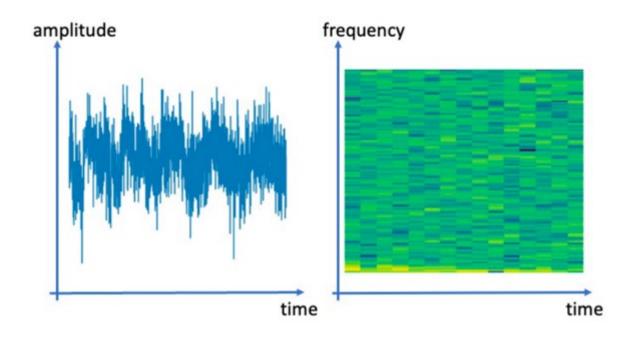


Figure 2.5: If the snapshot $\mathbf{z}^{(i)}$ is stored as a 512×512 RGB bitmap, we could use as features $\mathbf{x}^{(i)} \in \mathbb{R}^n$ the red-, green- and blue component of each pixel in the snapshot. The length of the feature vector would then be $n = 3 \times 512 \times 512 \approx 786000$.

Features of an Audio Recording.



label = song title

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 = A Cow



features:

duration of pregnancy

labels:

how much milk will it give next year?

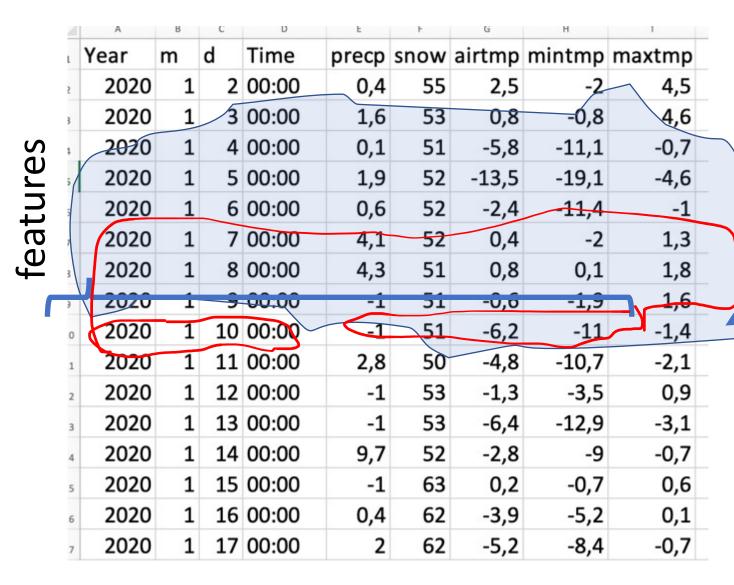
Datapoint = A Partial Differential Equation

features = a solution of the PDE

label = formula of PDE

datapoints, their features and labels are design choices!

A	В	C	υ	Ŀ	F	G	Н	1
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



data point

label

data point, features and label are design choices!

```
newdataset= somedata[somedata['date'] == '2021-06-01'];
print(newdataset)
         date
                time
                       temperature
   2021-06-01
               00:00
                               6.2
                               6.4
   2021-06-01
               01:00
   2021-06-01
               02:00
                               6.4
   2021-06-01
               03:00
                               6.8
   2021-06-01
               04:00
                               7.1
   2021-06-01
               05:00
                               7.6
   2021-06-01
               06:00
                               7.5
                               8.1
   2021-06-01
               07:00
   2021-06-01
               08:00
                              10.3
   2021-06-01
               09:00
                              12.8
10 2021-06-01
               10:00
                              15.0
11 2021-06-01
                              14.1
               11:00
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
                              13.3
               15:00
16 2021-06-01
               16:00
                              14.5
```

13.8

17 2021-06-01

17:00

Key Parameters of a Data Set

number *n* of features

number m of data points "sample size"

A	В	С	U	Ŀ	,	G	н	—
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	A.	20	108:00	ee p, &	ea y	ning,y	vith lo,s)	/tho <u>ŋ</u> 2

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
              00:00
  2021-06-01
  2021-06-01
              01:00
  2021-06-01 02:00
                                                   data point = some day at
                             6.8
  2021-06-01 03:00
  2021-06-01 04:00
                                                   FMI station
                             7.6
  2021-06-01 05:00
  2021-06-01 06:00
                             7.5
  2021-06-01
             07:00
                             8.1
                             10.3
8 2021-06-01
             08:00
  2021-06-01
             09:00
                                                   feature = nr of hourly observations
10 2021-06-01 10:00
11 2021-06-01
             11:00
12 2021-06-01
             12:00
                                                   want to predict maximum daytime
13 2021-06-01
             13:00
14 2021-06-01
              14:00
                                                   temperature
15 2021-06-01
             15:00
16 2021-06-01 16:00
                            14.5
17 2021-06-01
              17:00
                            13.8
```

missing relevant features bad for accuracy

```
newdataset= somedata[somedata['date'] == '2021-06-01'] :
print(newdataset)
        date
               time
                     temperature
              00:00
  2021-06-01
                             6.2
                                             data point = some day at
              01:00
  2021-06-01
                             6.4
  2021-06-01
              02:00
                             6.4
                                             FMI station
  2021-06-01
              03:00
                             6.8
                             7.1
  2021-06-01
             04:00
  2021-06-01
             05:00
                             7.6
  2021-06-01
              06:00
                             7.5
                             8.1
  2021-06-01
              07:00
                            10.3
  2021-06-01
              08:00
  2021-06-01
                            12.8
              09:00
                                             feature = hourly temp. 00:00 -
                            15.0
10 2021-06-01
              10:00
11 2021-06-01
              11:00
                            14.1
                                             15:00
              12:00
                            16.5
12 2021-06-01
13 2021-06-01
              13:00
                            13.6
                            14.2
14 2021-06-01
              14:00
                            13.3
15 2021-06-01
              15:00
                                             want to predict temp at 16:00
                            14.5
16 2021-06-01
              16:00
                            13.8
17 2021-06-01
              17:00
```

using irrelevant features wastes comp. resources

 regression: labels are numbers (temperature, distance, duration, ...)

 classification: labels are discrete-valued; represents category such as "Cat" vs. "No Cat"

• reg. /class. methods use diff. loss function (see later)

Label is Design Choice!

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

 Human agency and oversight:proper oversight mechanisms need to be ensured...

https://digital-strategy.ec.europa.eu/en/library/ethics-guidelines-trustworthy-ai

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.

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

```
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

Multi-Label Problems

data point with several different labels

the choice of label defines the ML task!

special case of multi-task learning

Multi-Label Regression.

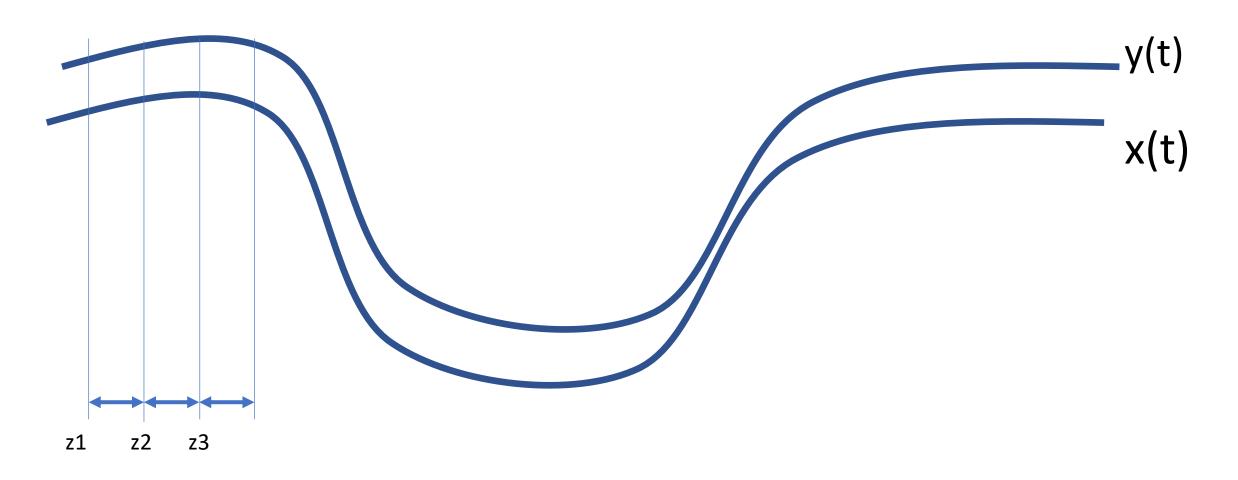
```
time
                     temperature
        date
                                    datapoint
  2021-06-01
              00:00
                            6.2
                            6.4
  2021-06-01
              01:00
                                     "2021-06-01 at some FMI station"
  2021-06-01
              02:00
                            6.4
                            6.8
  2021-06-01
              03:00
4 2021-06-01
              04:00
                            7.1
                            7.6
  2021-06-01
              05:00
6 2021-06-01
              06:00
                            7.5
  2021-06-01
              07:00
                            8.1
                                      label1 = tmp at 10:00
8 2021-06-01
              08:00
                           10.3
                           12.8
  2021-06-01
              09:00
10 2021-06-01
              10:00
                           15.0
                           14.1
11 2021-06-01
              11:00
                           16.5
12 2021-06-01
              12:00
13 2021-06-01
              13:00
                           13.6
                                      label2= tmp at 15:00
14 2021-06-01
              14:00
                           14.2
15 2021-06-01
                           13.3
              15:00
16 2021-06-01
                           14.5
              16:00
17 2021-06-01
              17:00
                           13.8
```

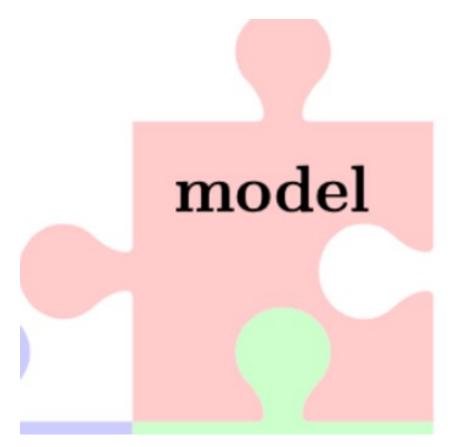
Multi-Label Classification.



 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

Effective Data Size m







Statisticians, like artists, have the bad habit of falling in love with their models.

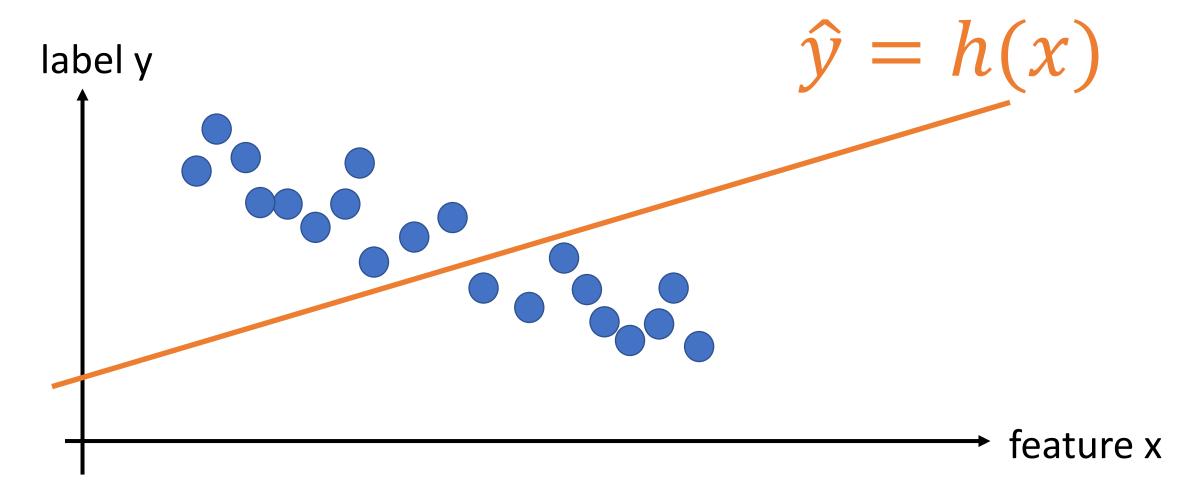
— George Е. Р. Вох —

AZ QUOTES

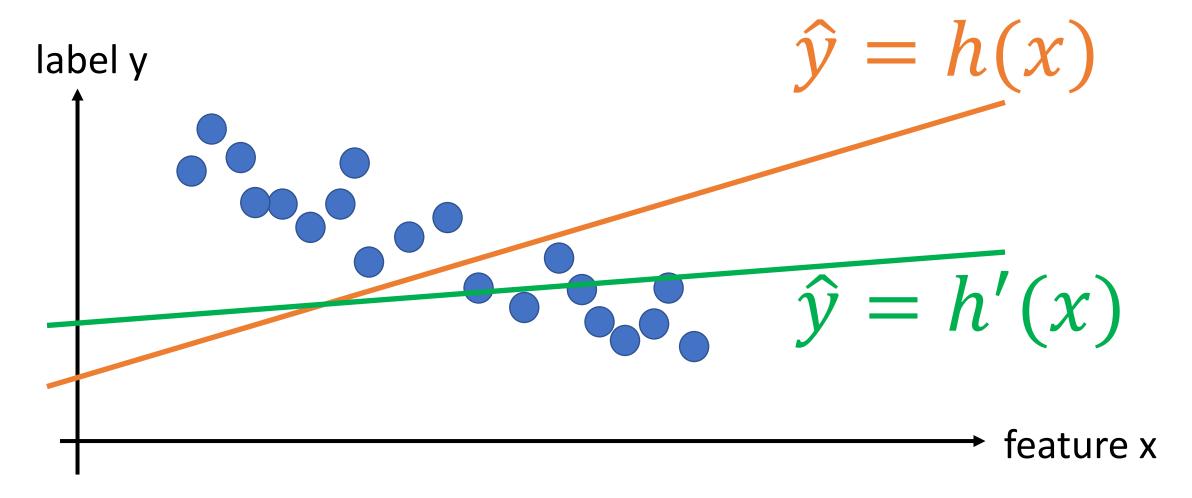
Machine Learning.

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

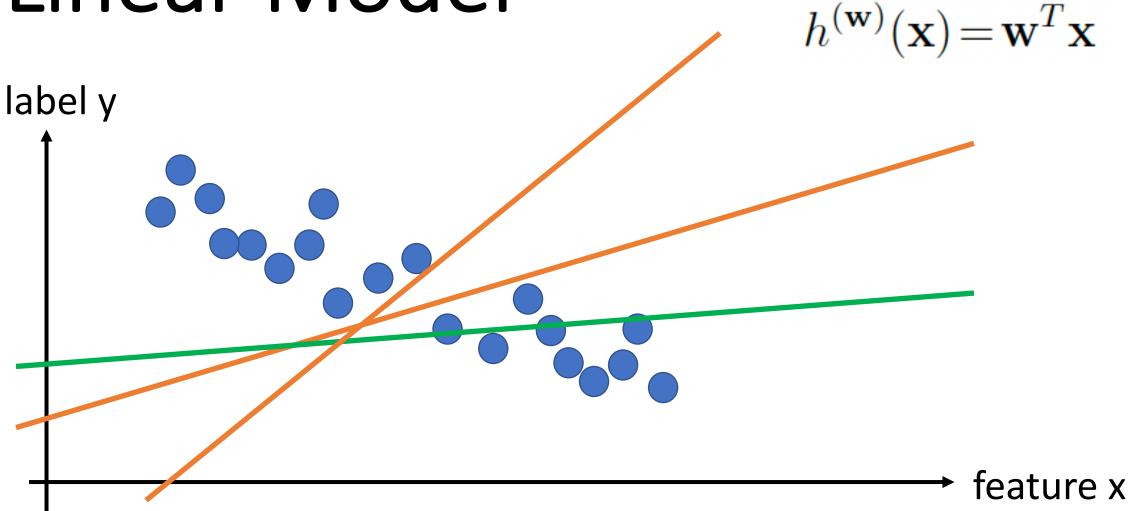
A Hypothesis.



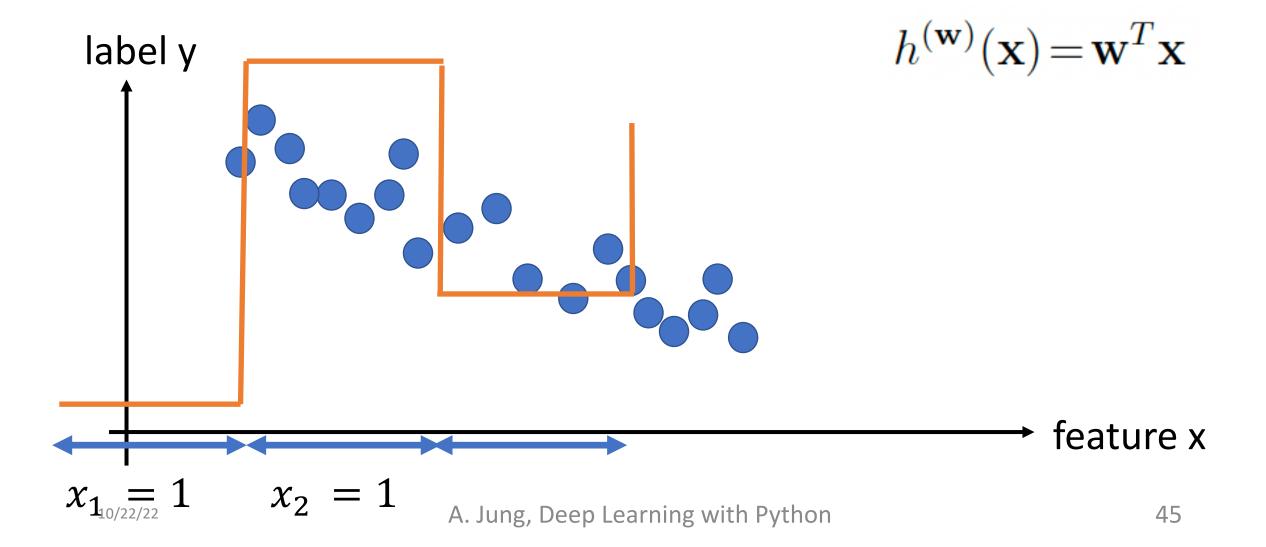
Model = Several Hypotheses.



Linear Model



Linear Model is Versatile!



Linear + Feature Map

feature map single feature x

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

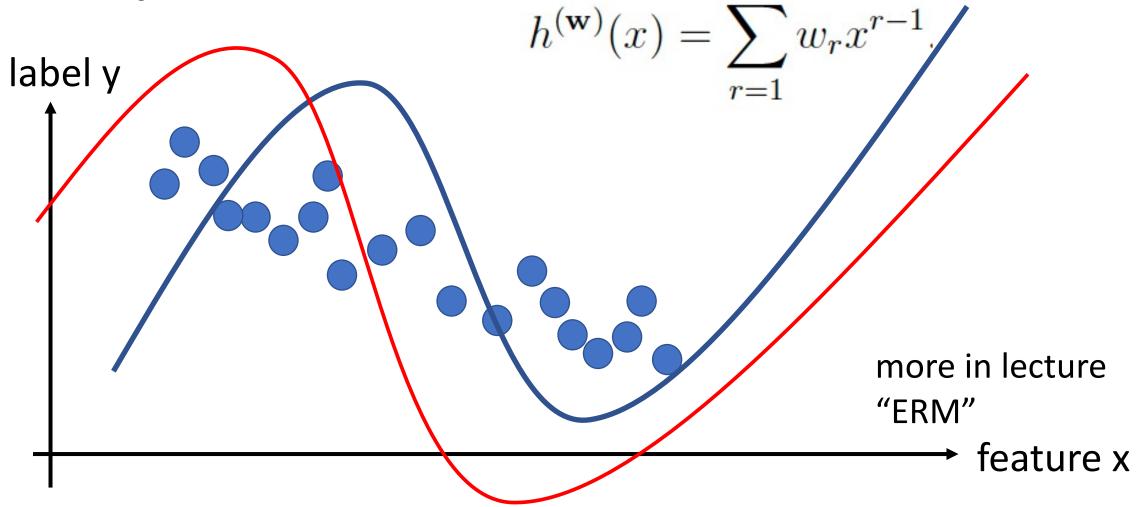
linear map

$$\begin{pmatrix} x_1 = \phi_1(x) \\ x_2 = \phi_2(x) \\ \vdots \end{pmatrix} \mathbf{w}^T \mathbf{x} = \sum_{j=1}^n w_j x_j$$

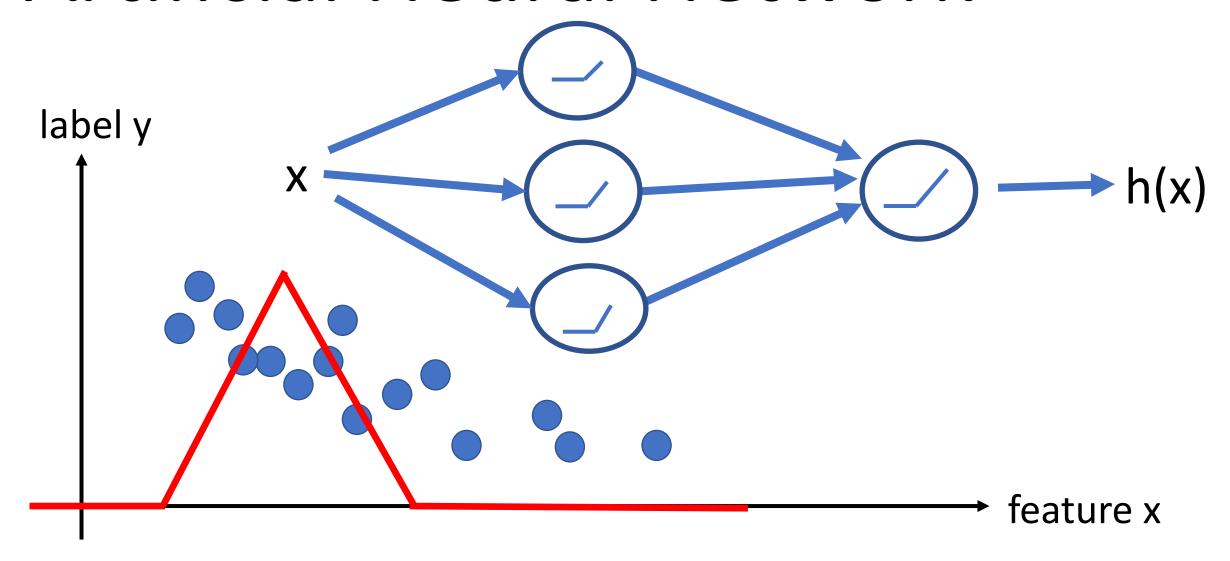
$$h(\mathbf{x})$$

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

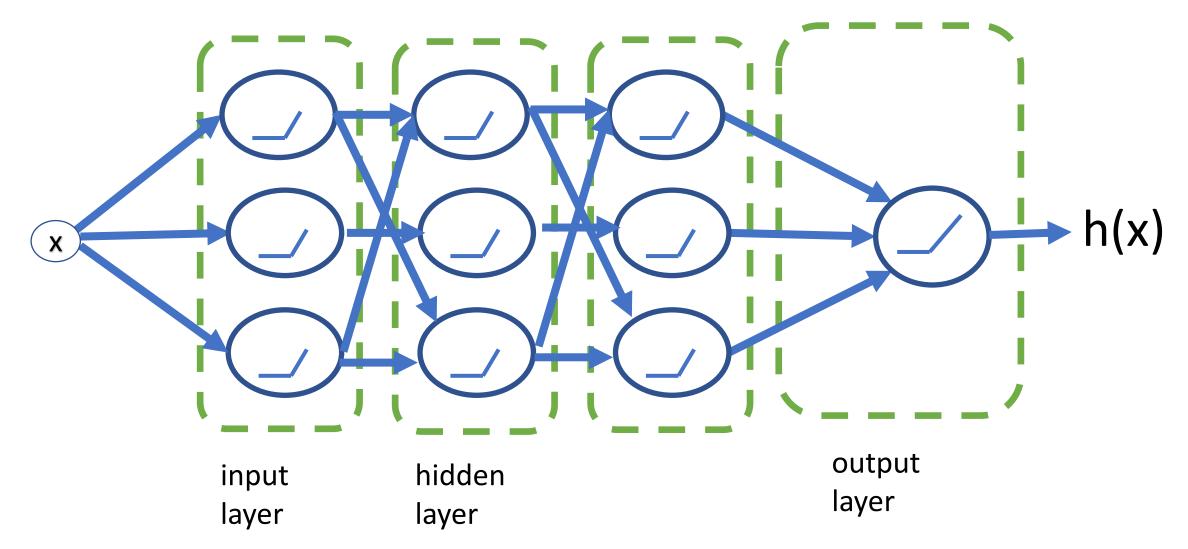
Polynomials



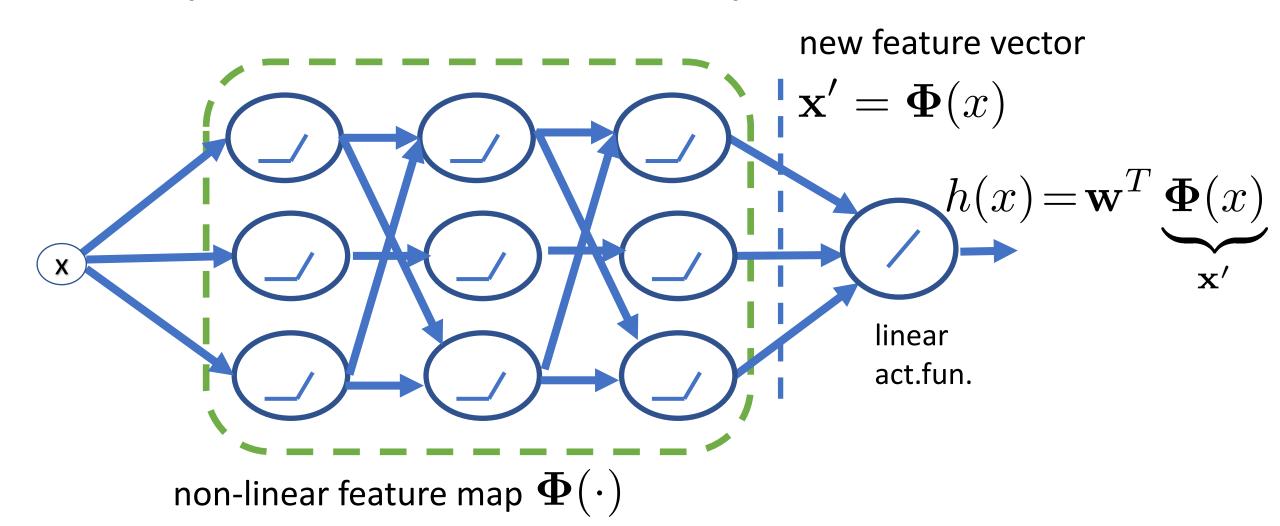
Artificial Neural Network



Deep ANN



Deep Net= Feature Map+Lin.Model



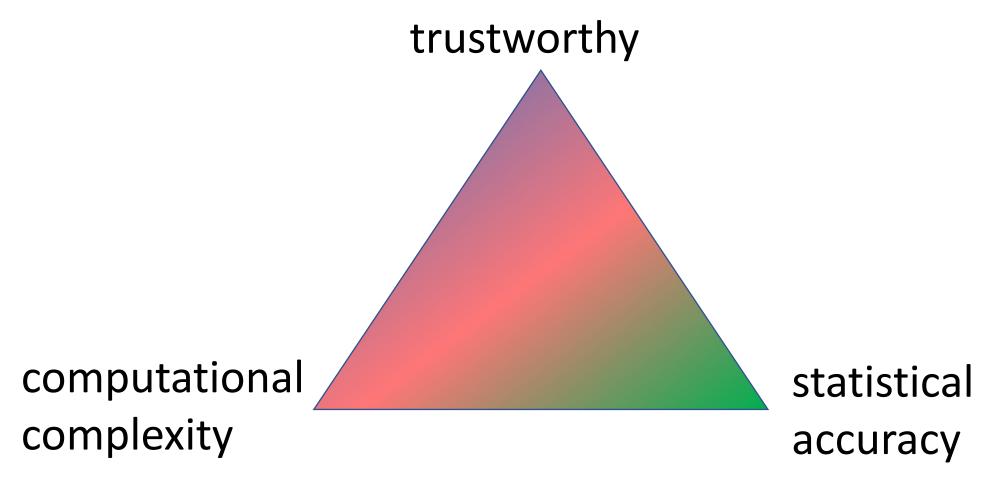
Which Model To Choose?

large to contain a suitable hypothesis

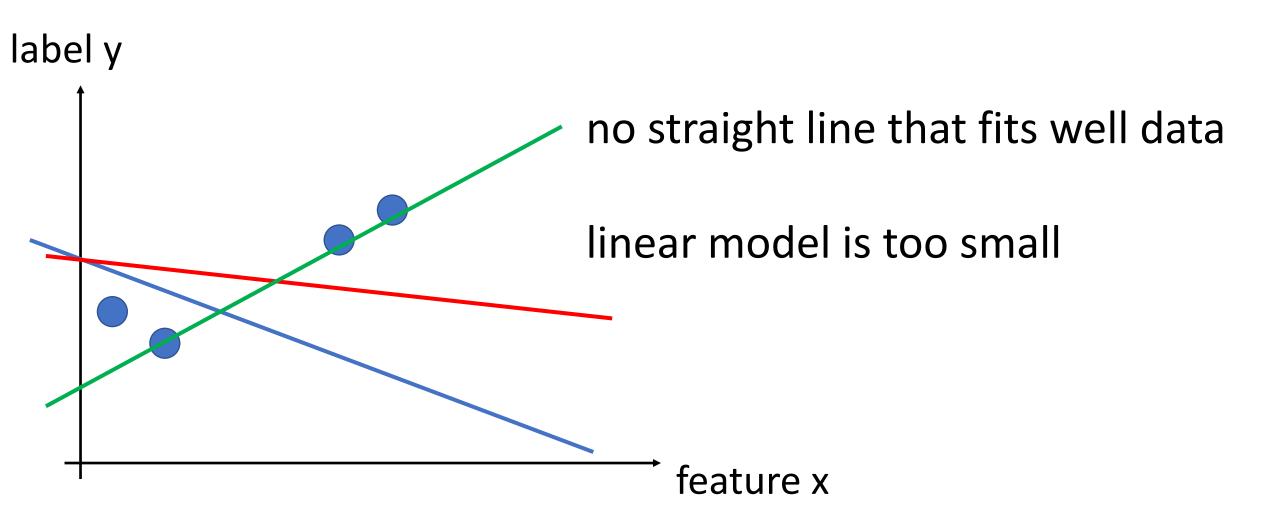
small to fit computational resources

simple or interpretable

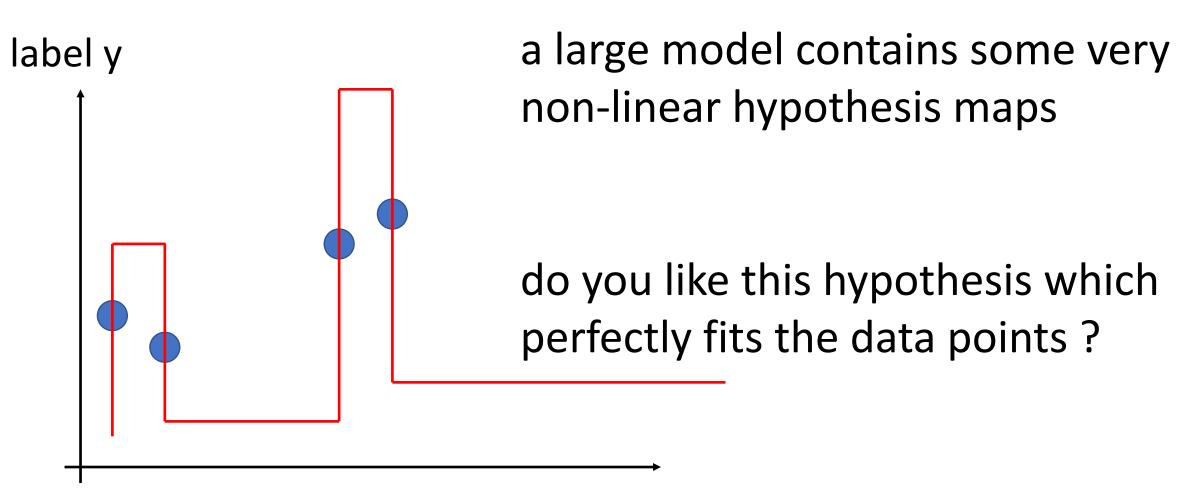
Design Choice: Model



Sufficiently Large



Sufficiently Small (Stat.)

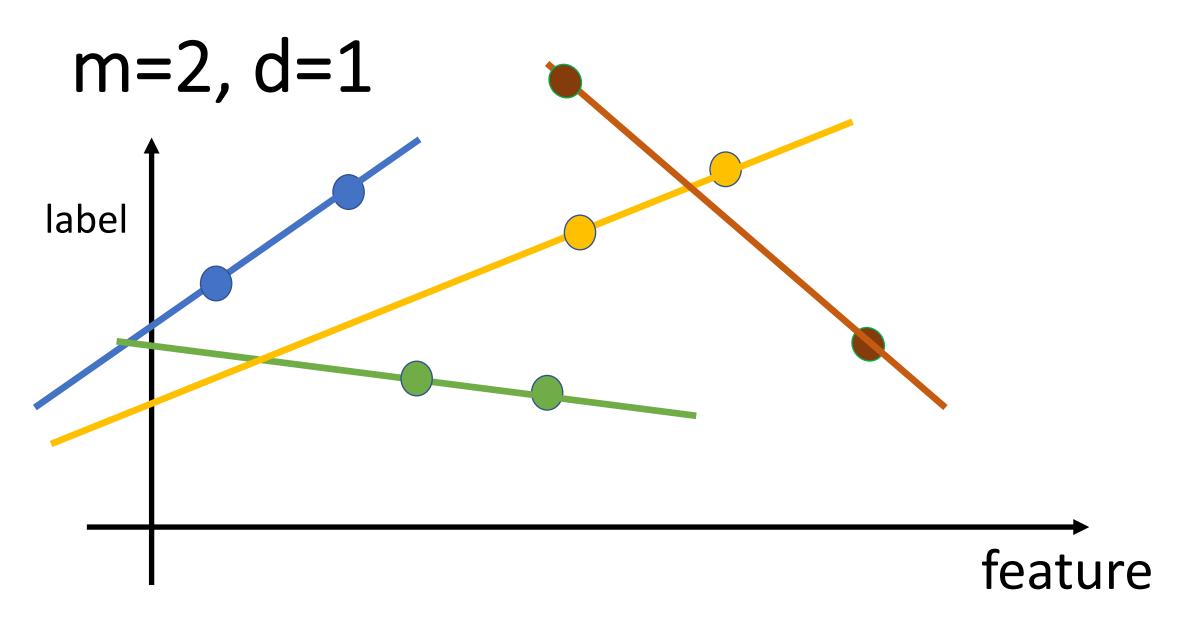


Sufficiently Small (Comput.)

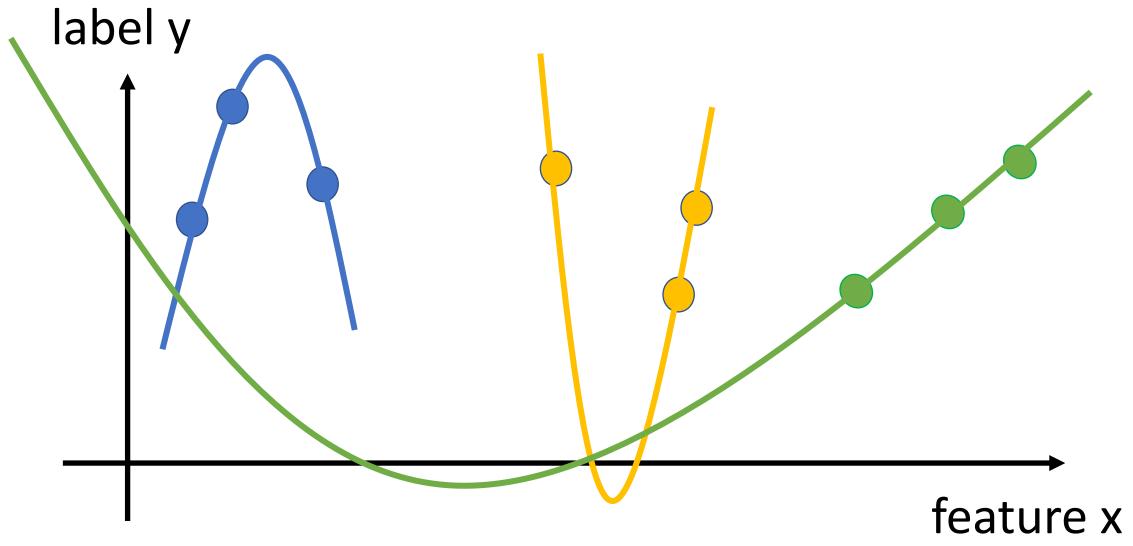
- consider linear regression using n features
- fit linear model on m > n datapoints
- need to invert "n by n" matrix!

Effective Model Size d

nr of data points that can be perfectly fit

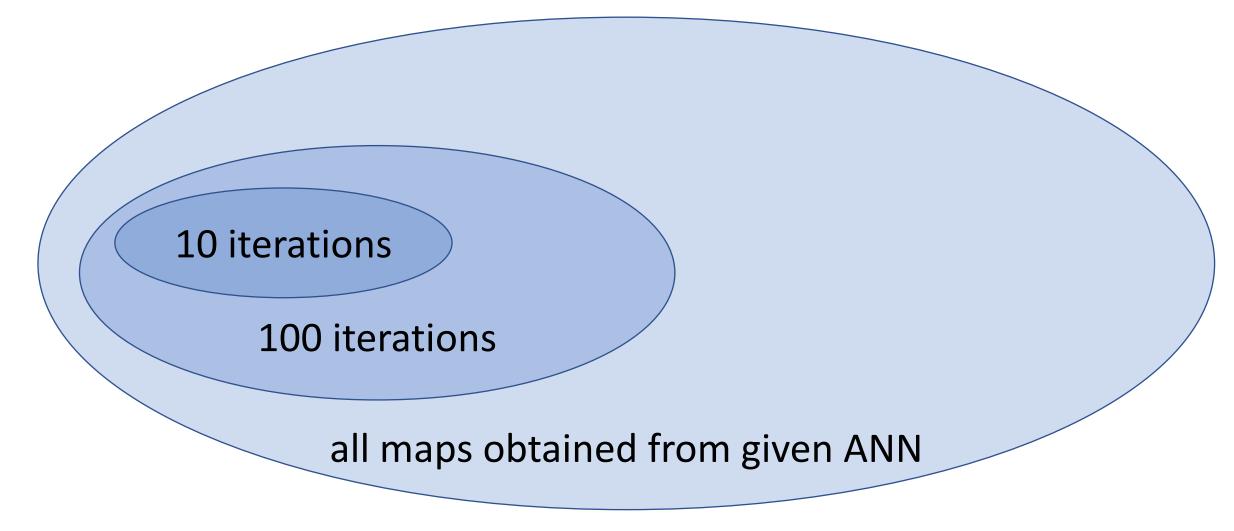


m=3, degree d=2 polynomial

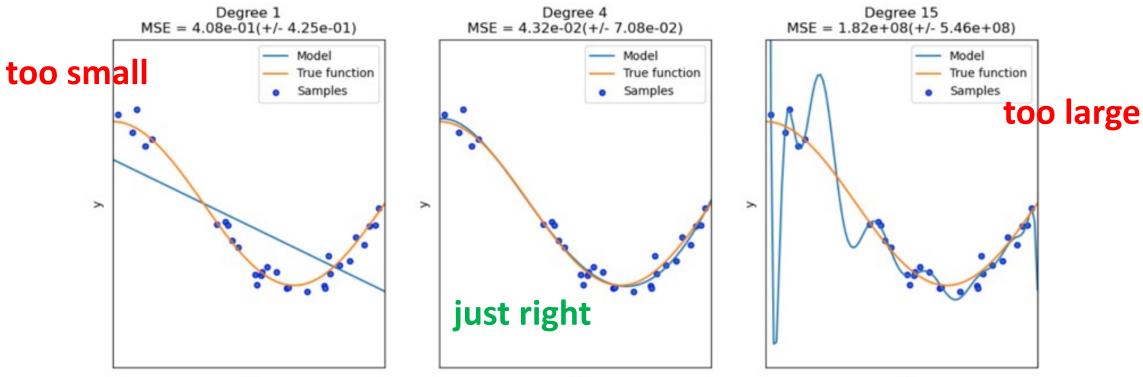


10/22/22

Effective Model Size d



Design Choice Relations



source: https://scikit-learn.org/stable/auto_examples/model_selection/plot_underfitting_overfitting.html

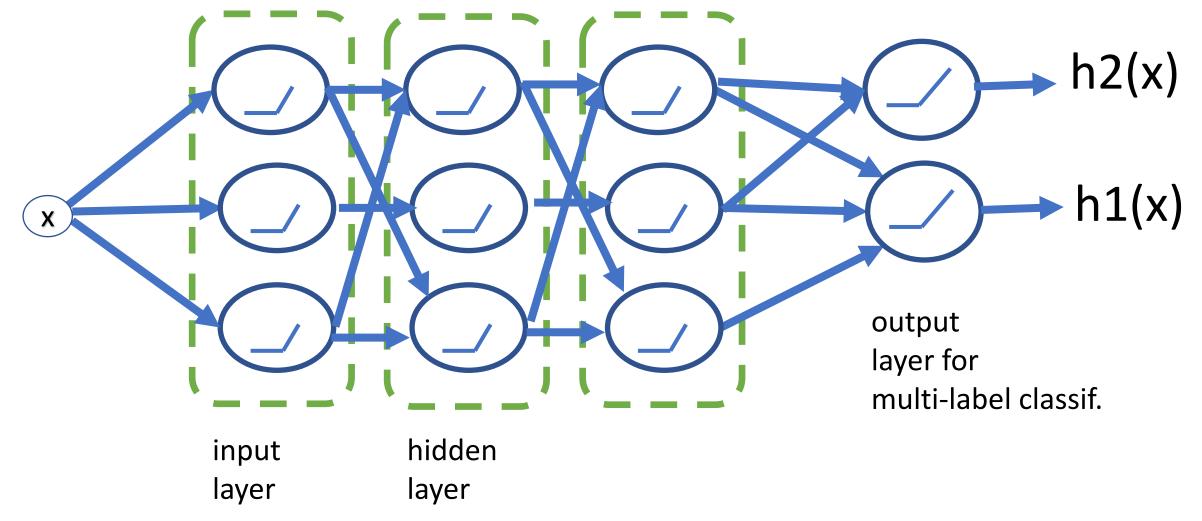
Alex' rule of thumb:

$$m >= 10 * d$$

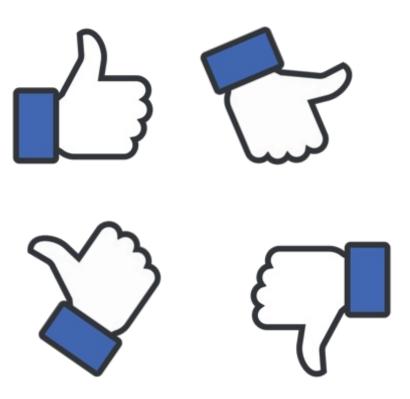
Design Choice Relations

- model must be suitable for data
- consider final layer of deep net
- for binary classif., cannot use ReLU or linear
- for regression, cannot use Sigmoid or SoftMax

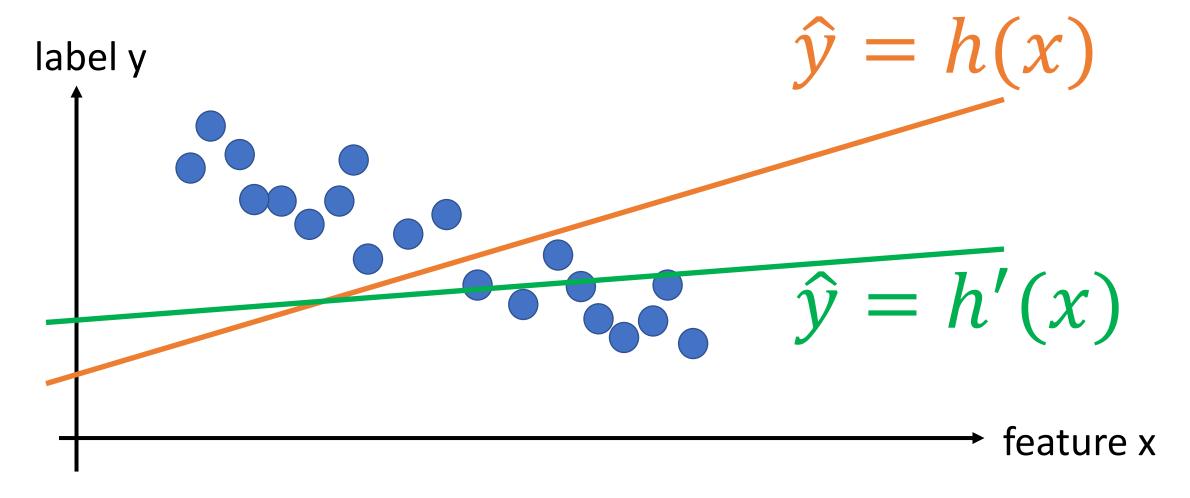
Design Choice Relations



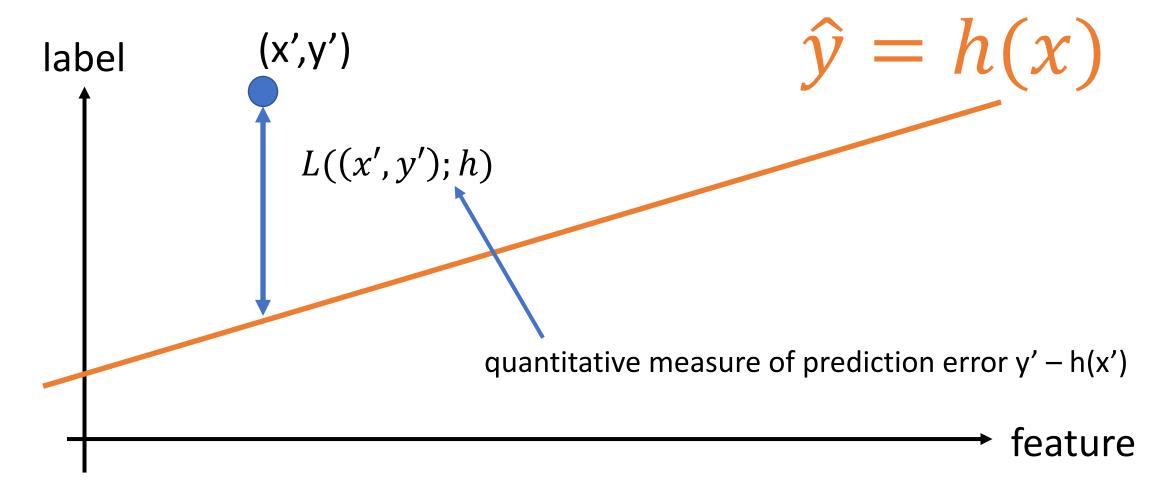




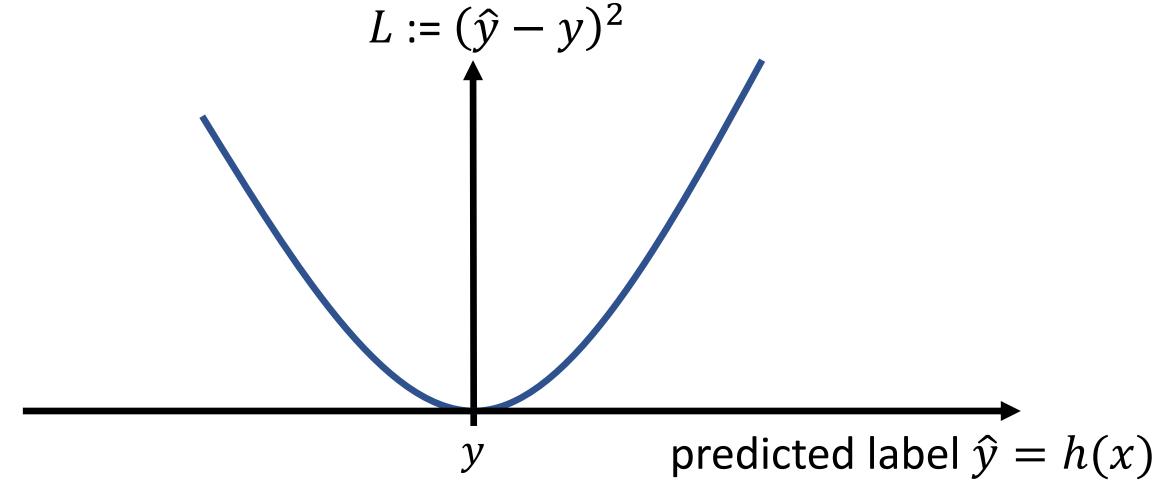
Which Hypothesis is Better?



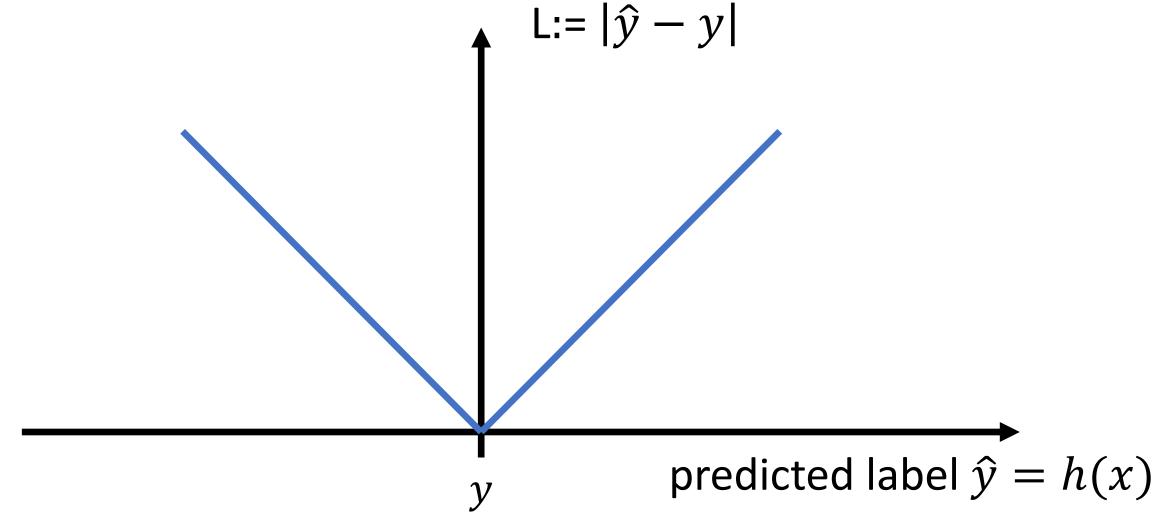
A Loss Function



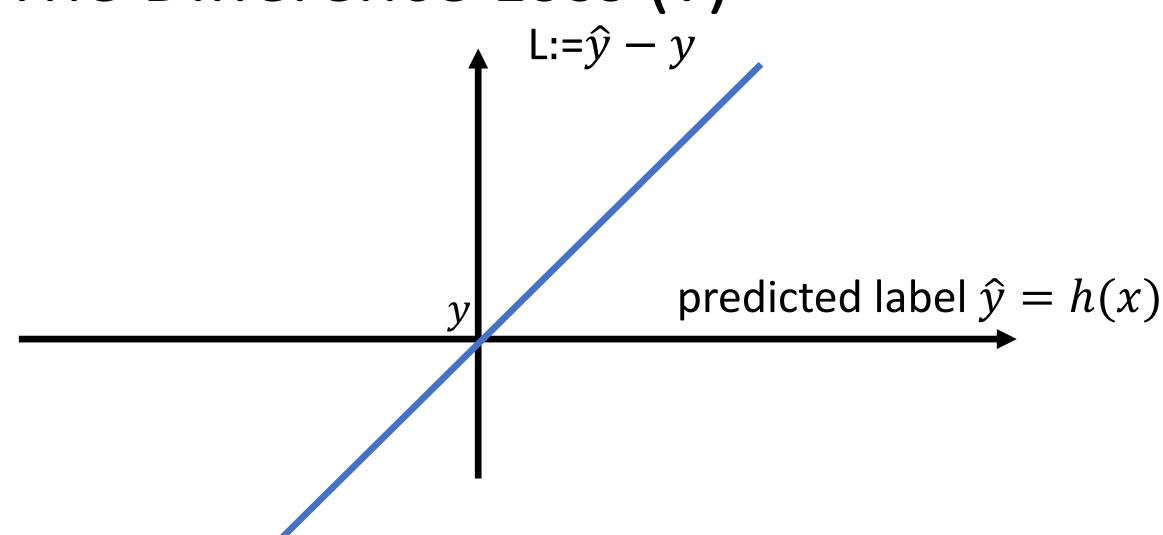
The Squared Error Loss



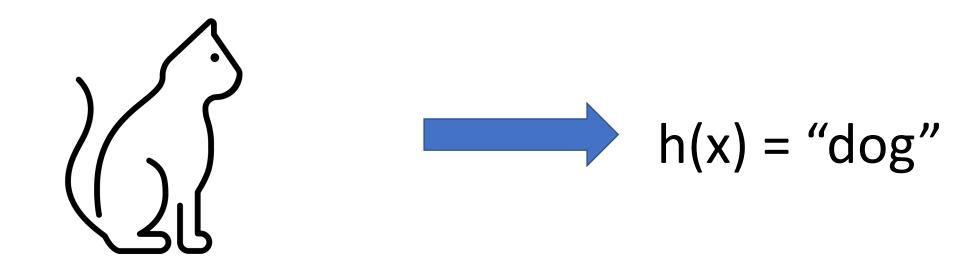
The Absolute Error Loss



The Difference Loss (?)



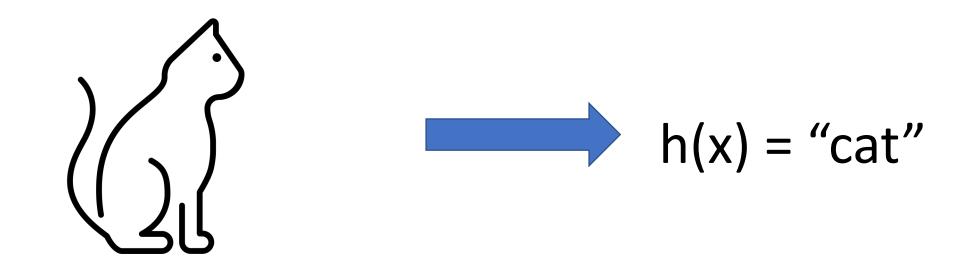
Loss Functions for Binary Classification



features x = pixels

Loss = 100

Loss Functions for Binary Classification



features x = pixels

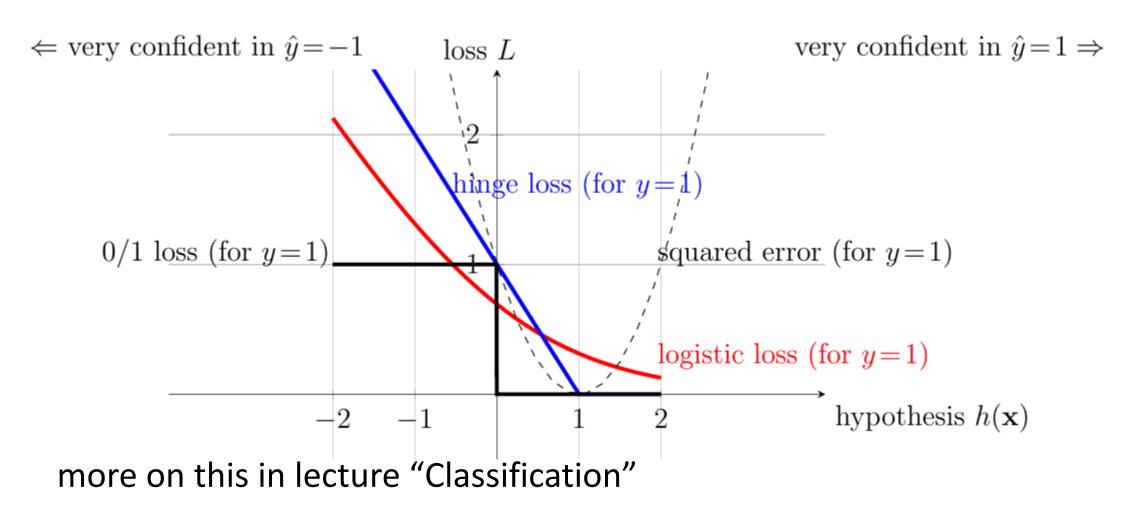
Loss = 0

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 \rightarrow "dog"
- use |h(x)| as confidence measure

Loss Functions for Binary Classification



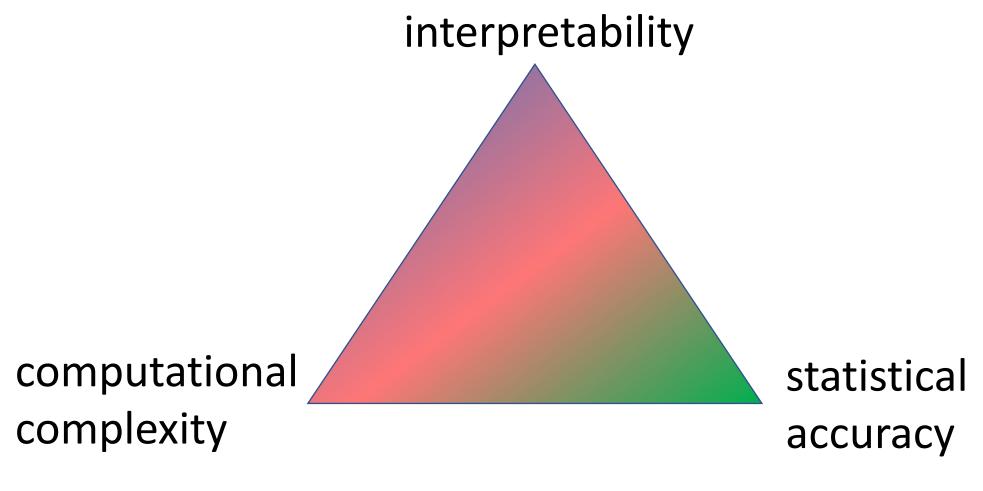
Which Loss Function?

- 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!

Design Choice: Loss



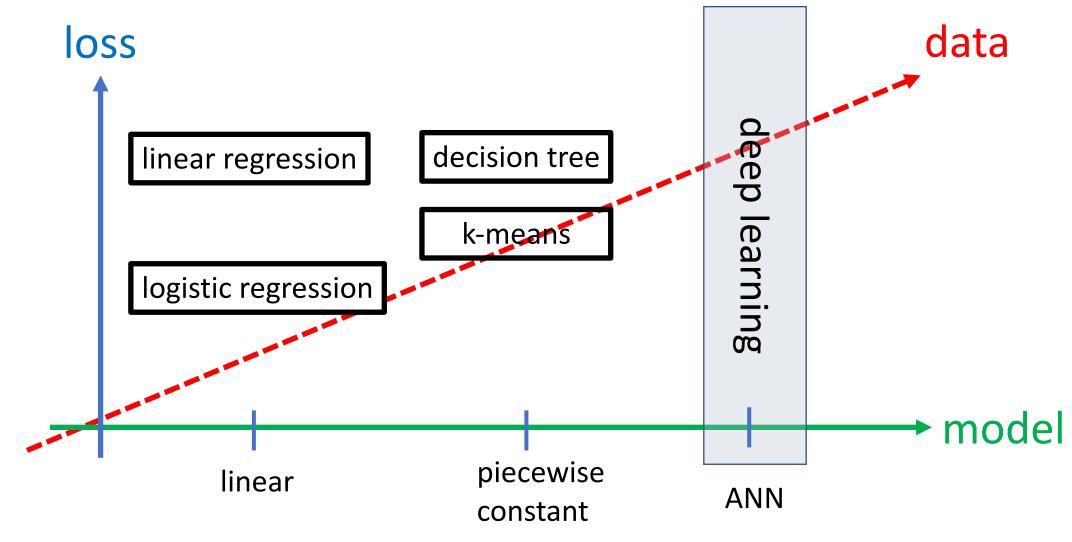
Main Components of ML

data

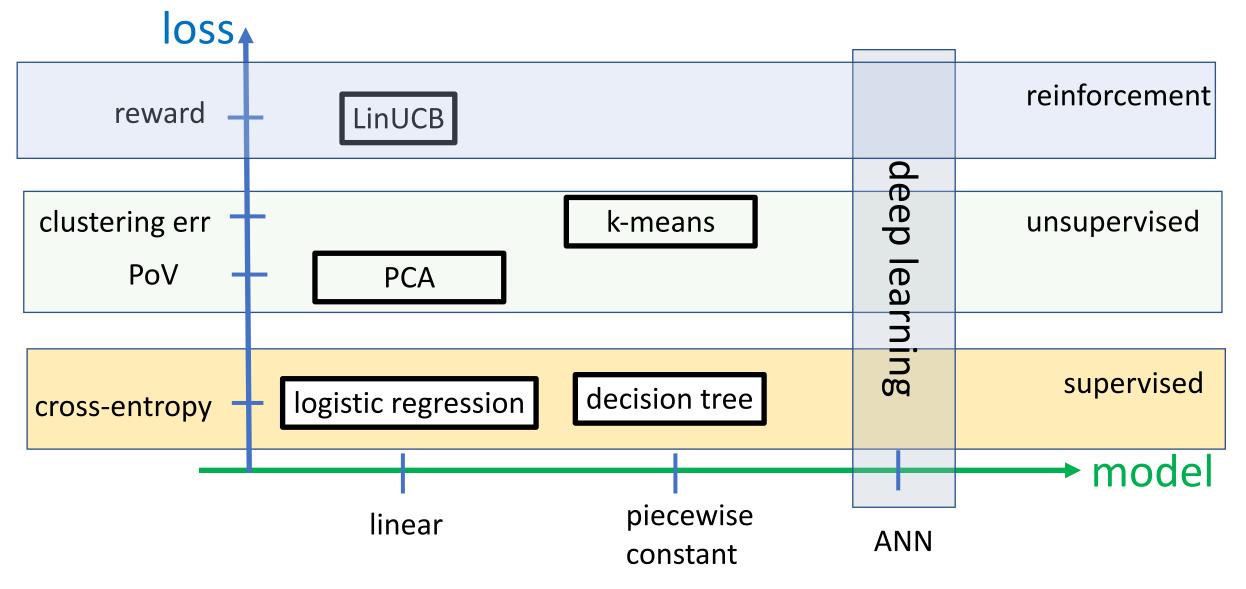
model

• loss

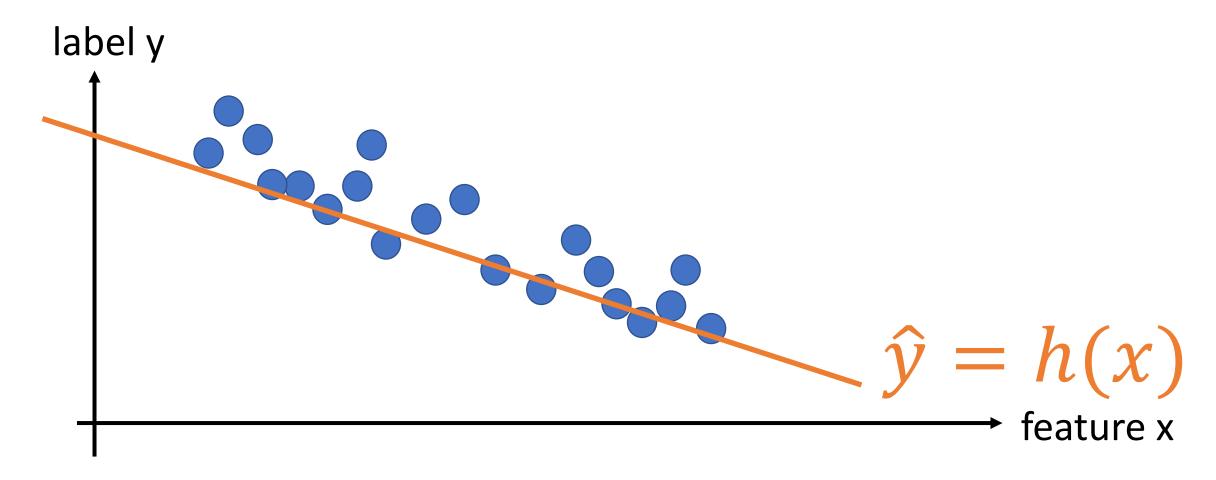
Landscape of ML Methods



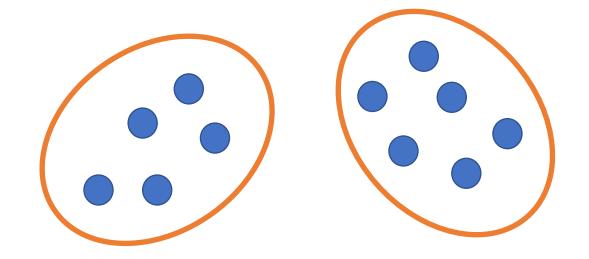
Three Main Flavours of ML



Supervised Learning



Unsupervised Learning



label = cluster index (1 or 2)

clustering methods (such as "k-means") do not require true label for any data point!

Reinforcement Learning

features = on-board camera video

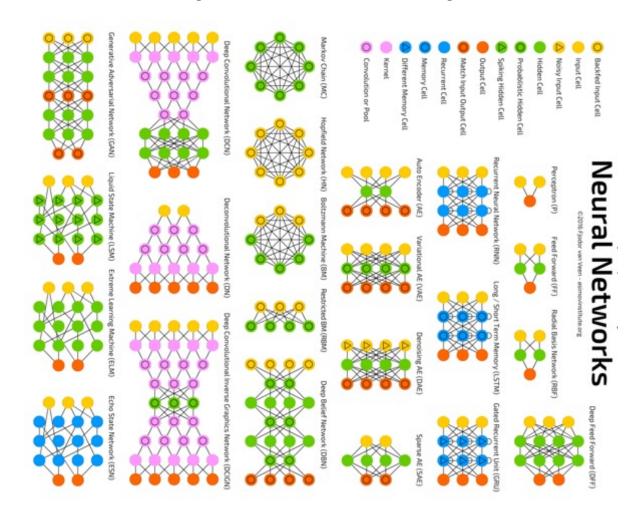
label = "optimal steering

direction"



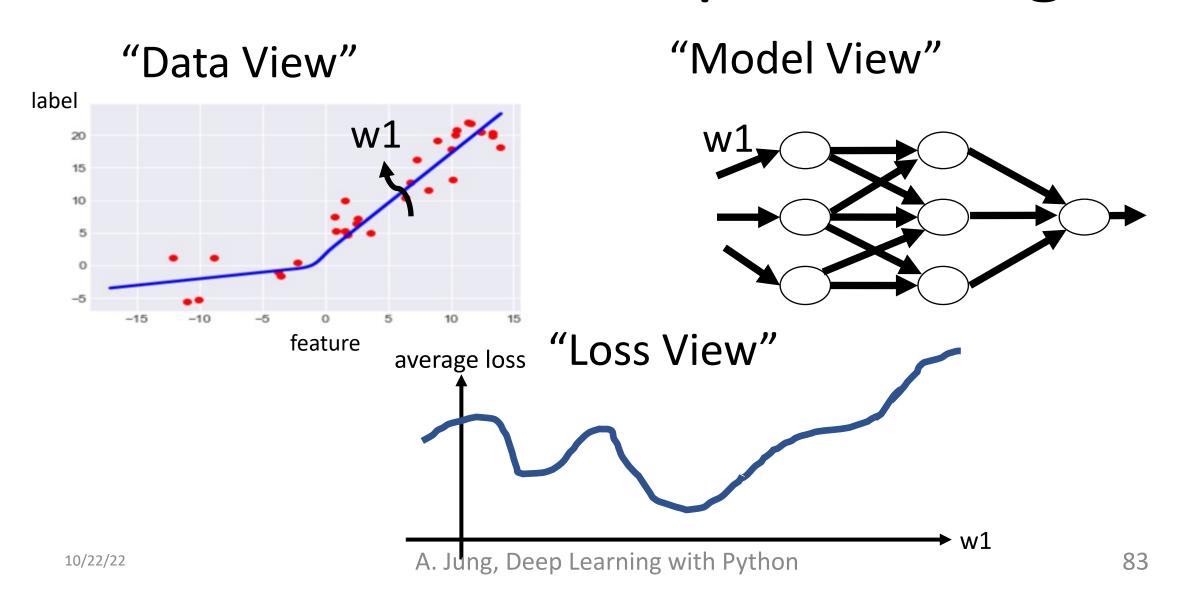
not covered in this course!

Landscape of Deep Learning



https://www.asimovinstitute.org/neural-network-zoo/

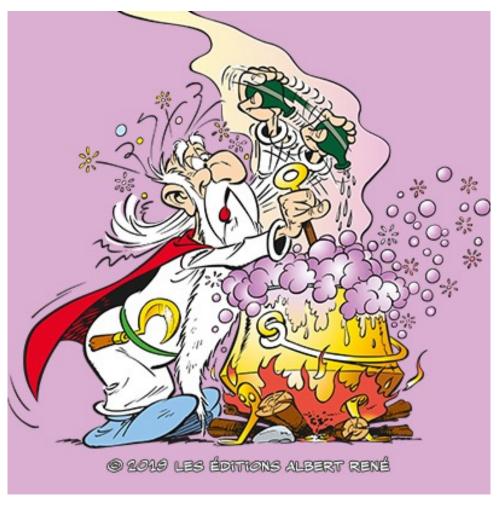
Three Views on Deep Learning



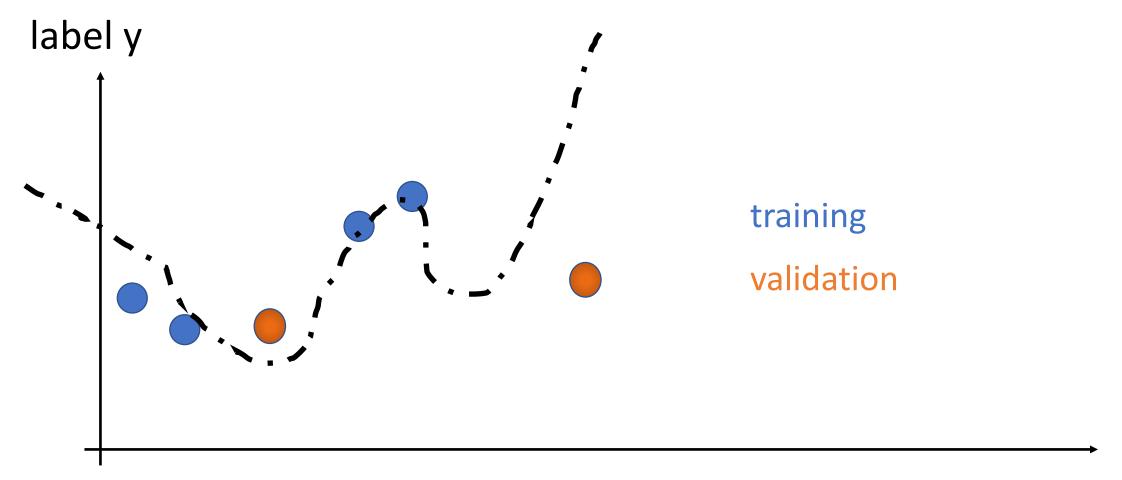
Deep Learning Python code often follows the following pattern:

- 1. choose/load data
- 2. choose/build model (ANN structure)
- 3. choose/construct loss function
- 4. tune model parameters to min. loss

Putting Things Together

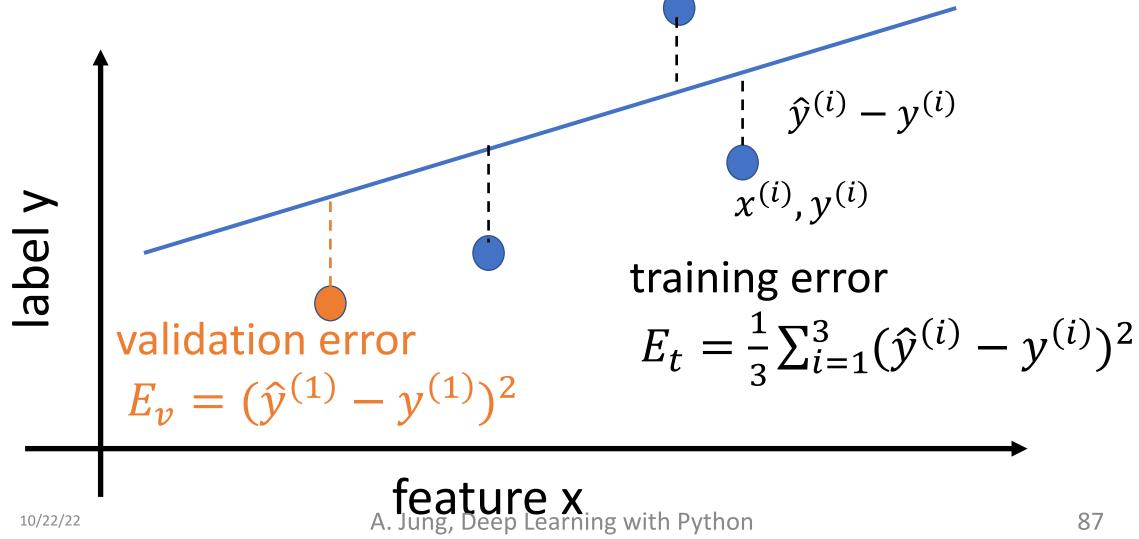


Train and Validate!

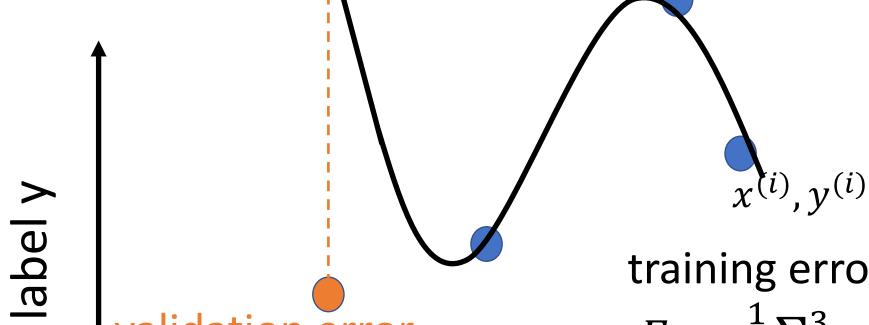


feature x

Train and Validate Model 1



Train and Validate Model 2



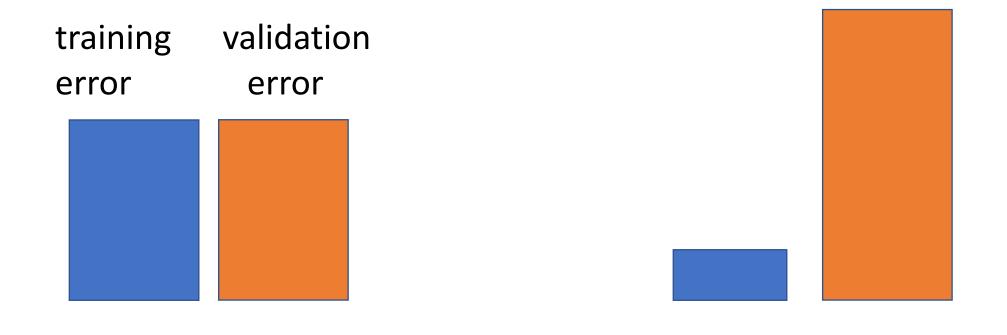
$$E_{v} = (\hat{y}^{(1)} - y^{(1)})^{2}$$

training error

$$E_t = \frac{1}{3} \sum_{i=1}^{3} (\hat{y}^{(i)} - y^{(i)})^2$$

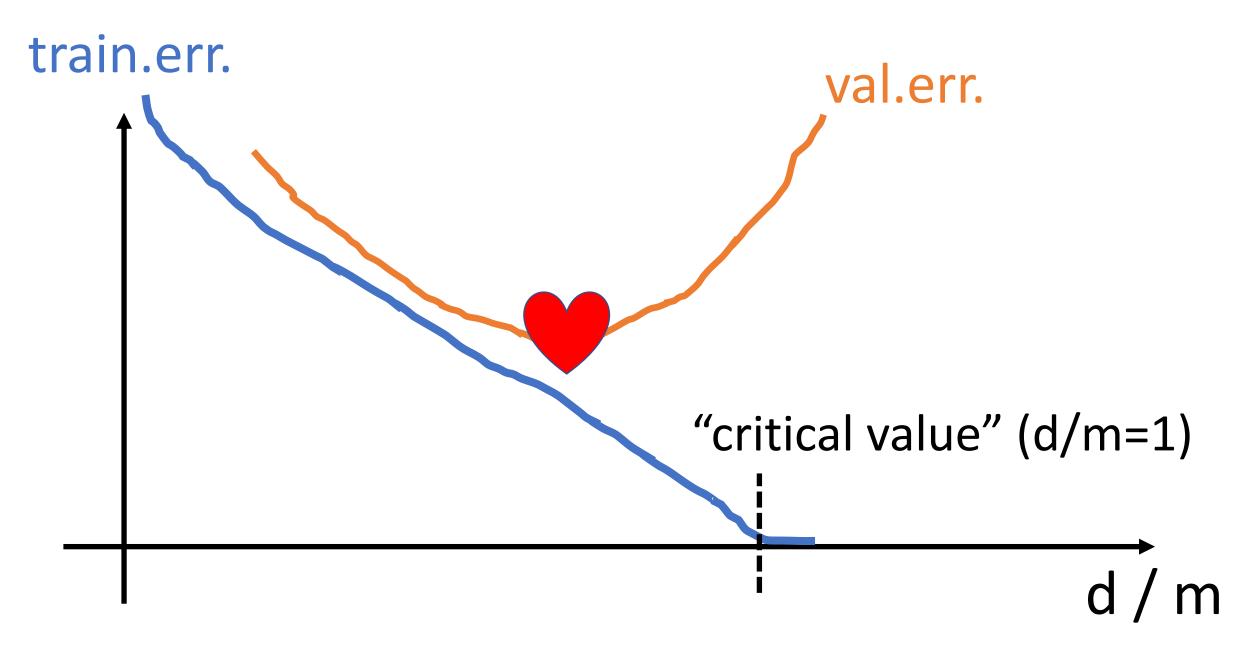
feature x

Choose Model via Val. Error

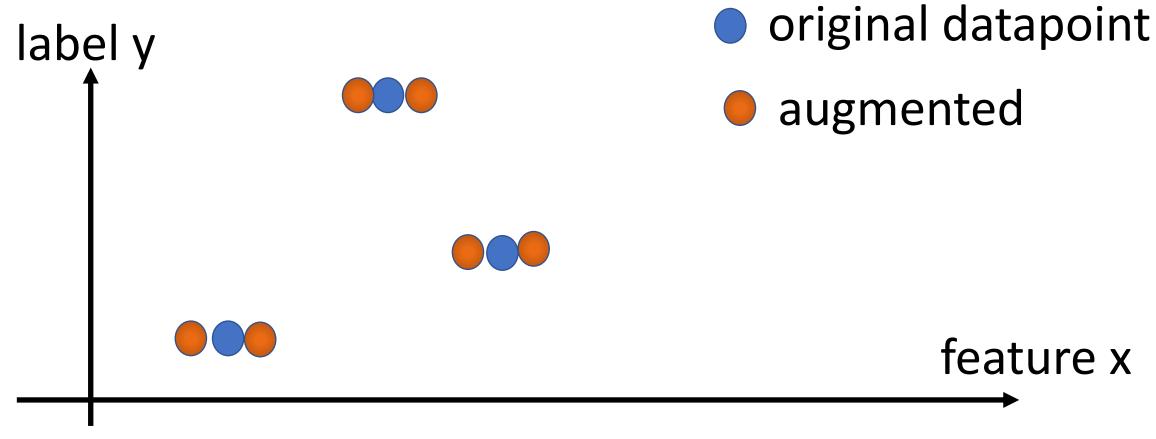


model 1: ANN 1 layer

model 2: ANN 3 layers

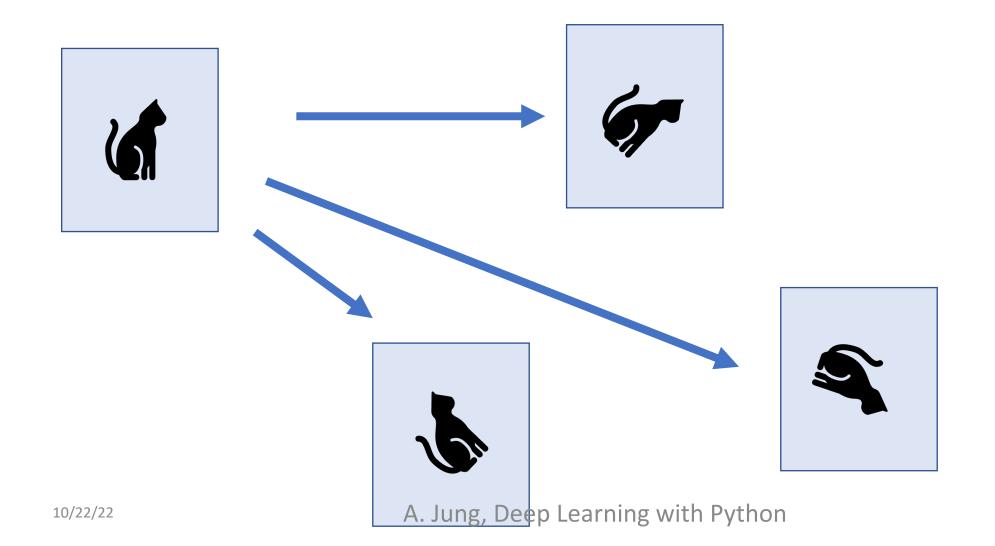


increasing effective data size m



we have increased the dataset by factor 3!

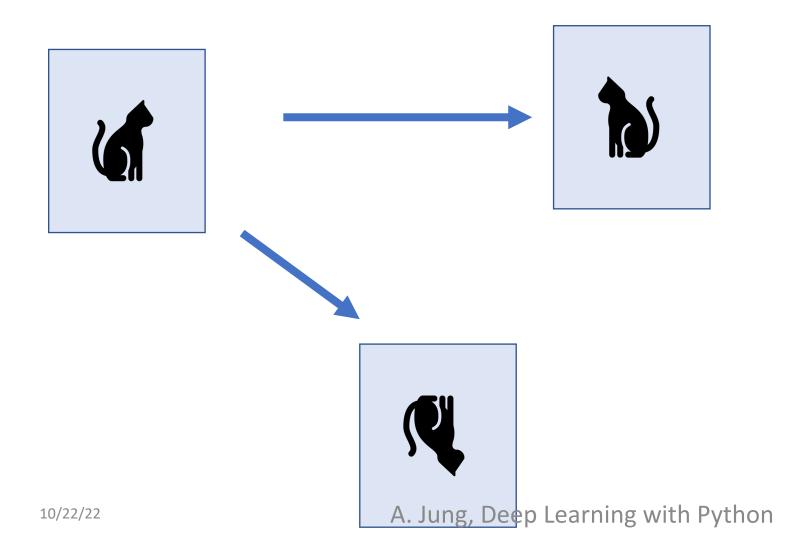
rotated cat image is still cat image



92

flipped cat image is still cat image

93



Data Augmentation via Regularization

label y

h(x)

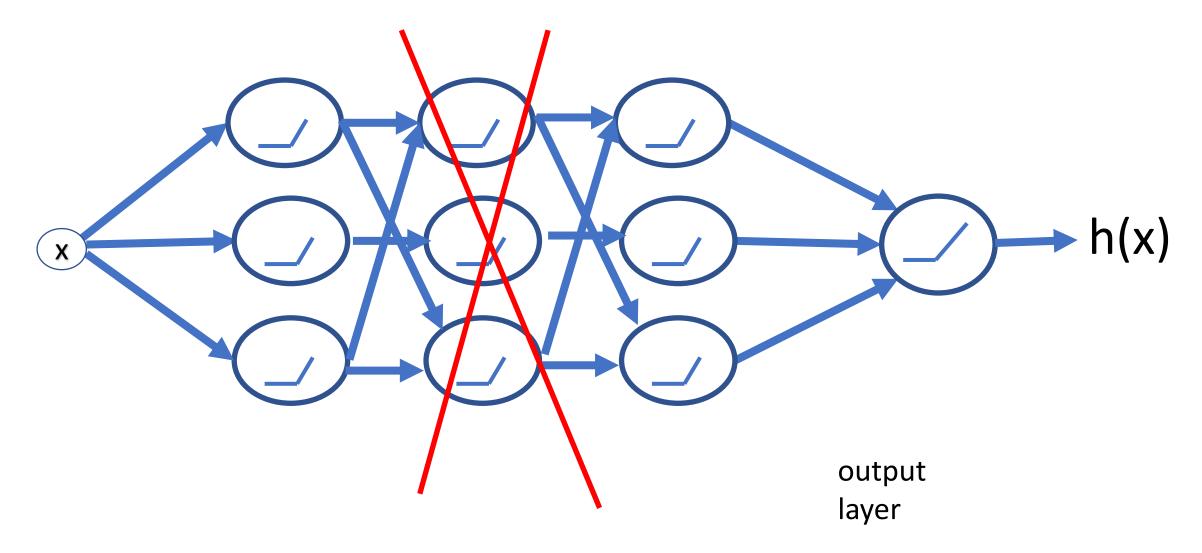
- orig. datapoint
- "perturbed"datapoint

$$\frac{1}{m} \sum_{i=1}^{m} L((x^{(i)}, y^{(i)}), h) + \lambda \mathcal{R}(h)$$

see Chapter 7.3 of mlbook.cs.aalto.fi

feature x

decrease model size d



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 map h(.) such that h(x) $\approx y$
- ML model = comp. tractable subset of possible maps h(.)
- ML quantifies prediction error y-h(x) with a loss function

What's Next?

Zoom Support Session 27.10 at 14:00 pm

 Support Session Fr. 12-16:00 pm hall AS4 in TUAS building (Maarintie 8)

join our Slack!