11. Review of Machine Learning Methods and Applications

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"A review of the first ten lectures for the mid-term exam."

MANE 4962 and 6962

Outline: Five methods & three tasks

unsupervised

Machine learning methods:

- kNN
- k-means
- Linear regression
- Logistic regression
- Neural Networks

supervised vs unsupervised

Machine learning tasks:

- Classification
- Regression
- Clustering

Supervised

cluster

Inputs, outputs, and mathematics of ML

Inputs

- The input is typically an n-dimensional vector which quantify what we know about the problem. The components of the vector are termed features. A set of features are a representation of the data.

Outputs

- The output is a dependent variable, commonly known as a target.
- Targets are discrete variables, if we want to identify/categorize/classify something. (classification task)

  0, 1, 2, 3, . . .
- Targets are continuous variables, if we want to predict/regress/estimate something. (regression task)

Linear algebra

- Vector and matrix algebra

Optimization

- Gradient Descent and its variants

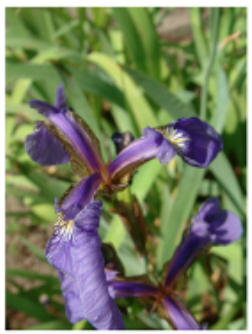
k-Nearest Neighbors (kNN)

K = 3

memorize/instance-based

P = 2

1. Find all the nearest neighbors using a distance metric, $d(\underline{x}, \underline{x}') = ||\underline{x} - \underline{x}'||_p$ the training
2. For classification, return the average/majority class as the class label.
3. For regression, return local interpolation of the targets of the nearest neighbors.

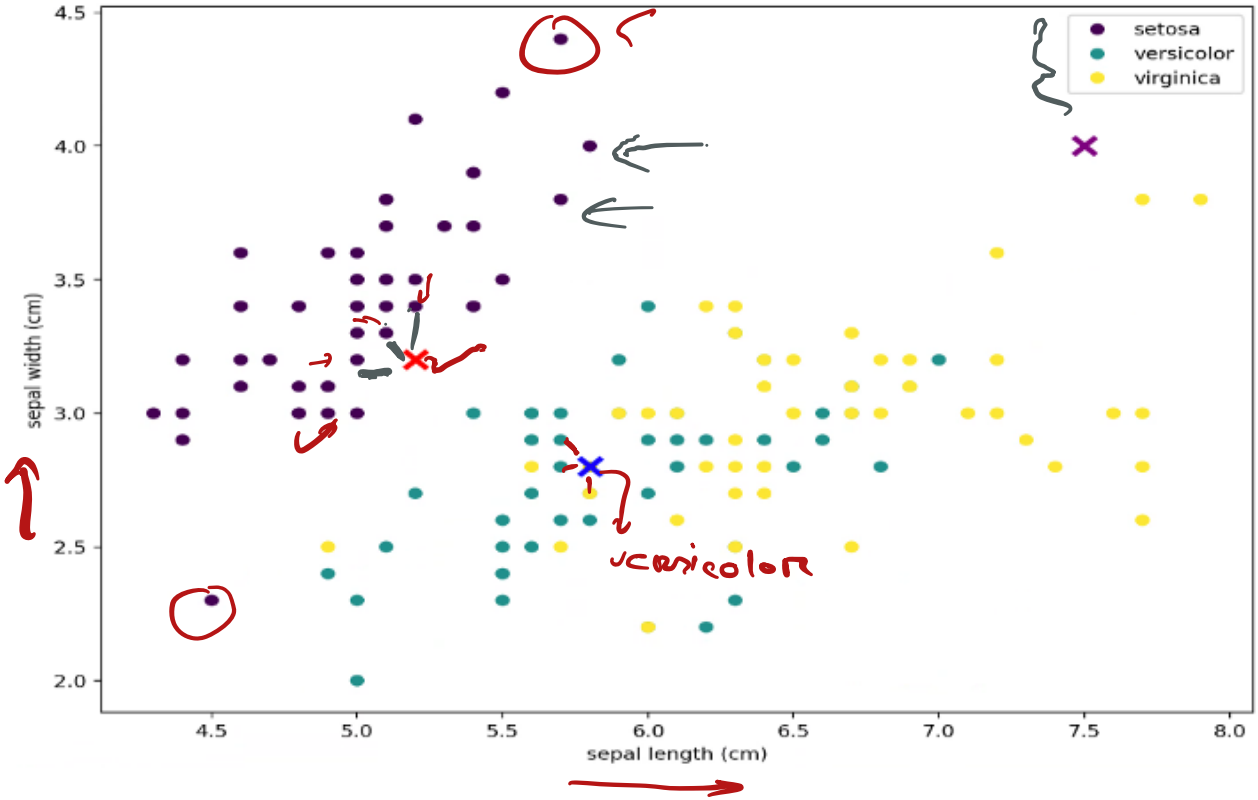


Iris setosa

Iris versicolor

Iris virginica

iris



A simple implementation of K-NN

```
class My_KNNClassifier:
    def __init__(self, k=3):
        self.k = k
    def fit(self, X_train, y_train):
        self.X_train = X_train
        self.y_train = y_train
    def predict(self, X_test):
        predictions = []
        for i in range(X_test.shape[0]):
            predictions.append(self._knn_classifier(X_test[i]))
        return predictions
    def _knn_classifier(self, X_test):
        distances, targets = [], []
        for i in range(self.X_train.shape[0]):
            distance = np.linalg.norm(self.X_train[i]-X_test)
            distances.append([distance, i])
        distances = sorted(distances)
        for i in range(self.k):
            index = distances[i][1]
            targets.append(self.y_train[index])
        return max(targets, key=targets.count)
model = My_KNNClassifier()
model.fit(X_train, y_train)
preds = model.predict(X_test)
print(accuracy_score(y_test, preds))
```

X_{train}, Y_{train} fit

predict

Norm, p = 2

Hyperparameter

0.92

Check notebook for Lecture 4.

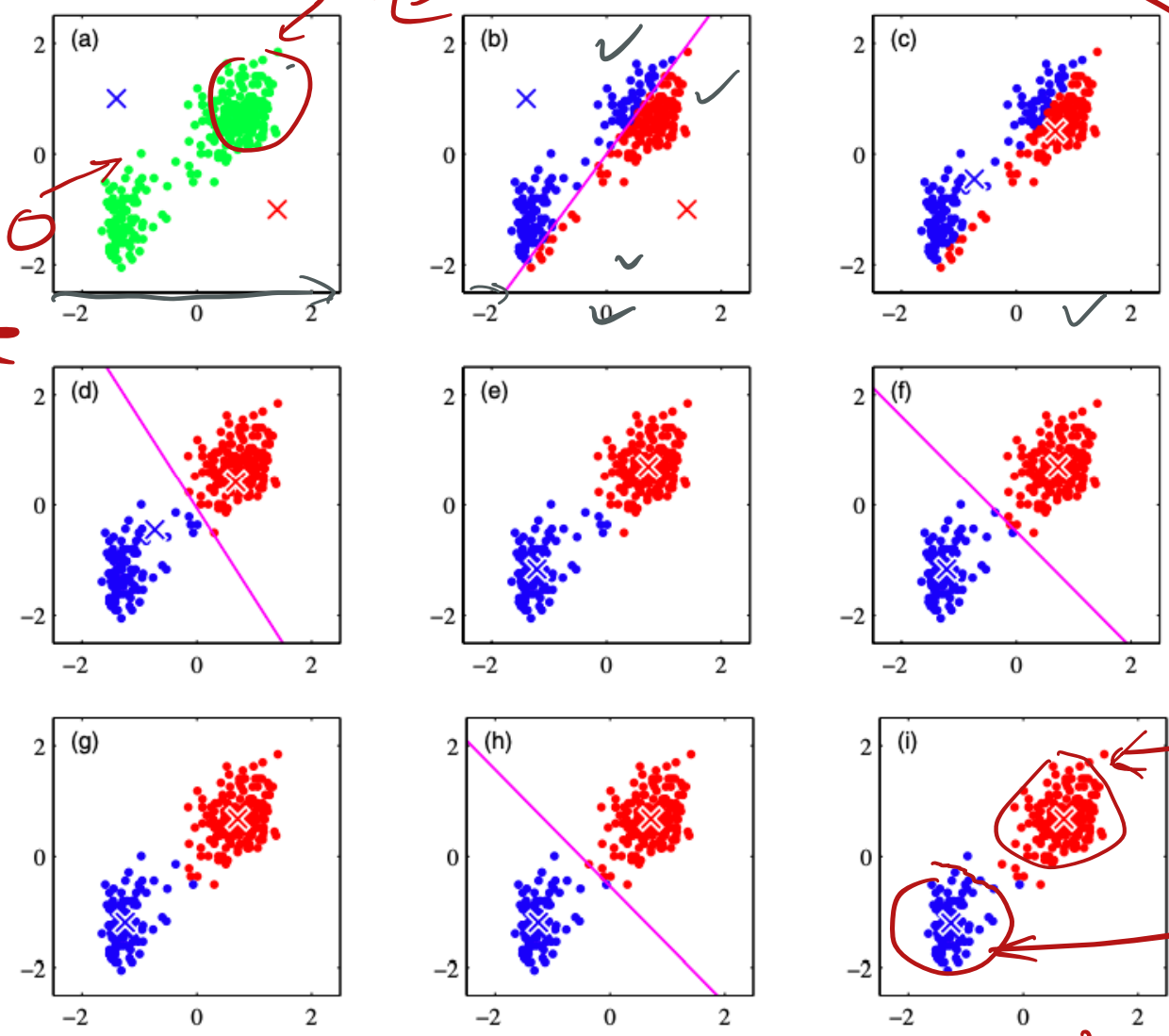
k-means clustering

1. Initiate centers

2. Calculate distances

3. Assign points to the center

stopping centers are staying



Clustering is not the same as classification so do not use accuracy to evaluate clustering.
Use silhouette scores.

A simple implementation of k-means

Supervised → KNN Kmeans ← unsupervised

```
class KMeans:
    def __init__(self, k):
        self.k = k
        self.cluster_labels = None
    def fit(self, X):
        self.centroids = X[np.random.choice(X.shape[0], self.k, replace=False), :]
        self.cluster_labels = np.arange(self.k)
        while True:
            distances = np.array([np.linalg.norm(X - centroid, axis=1) for centroid in self.centroids])
            self.clusters = np.argmin(distances, axis=0)
            new_centroids = np.array([X[self.clusters == i, :].mean(axis=0) for i in range(self.k)])
            # check convergence
            if np.array_equal(new_centroids, self.centroids):
                break
            else:
                self.centroids = new_centroids
    def predict(self, X):
        distances = np.array([np.linalg.norm(X - centroid, axis=1) for centroid in self.centroids])
        return self.cluster_labels[np.argmin(distances, axis=0)]
```

(X, y) , X

Check notebook for Lecture 5.

Scikit → max_iteration

Linear Models and NN

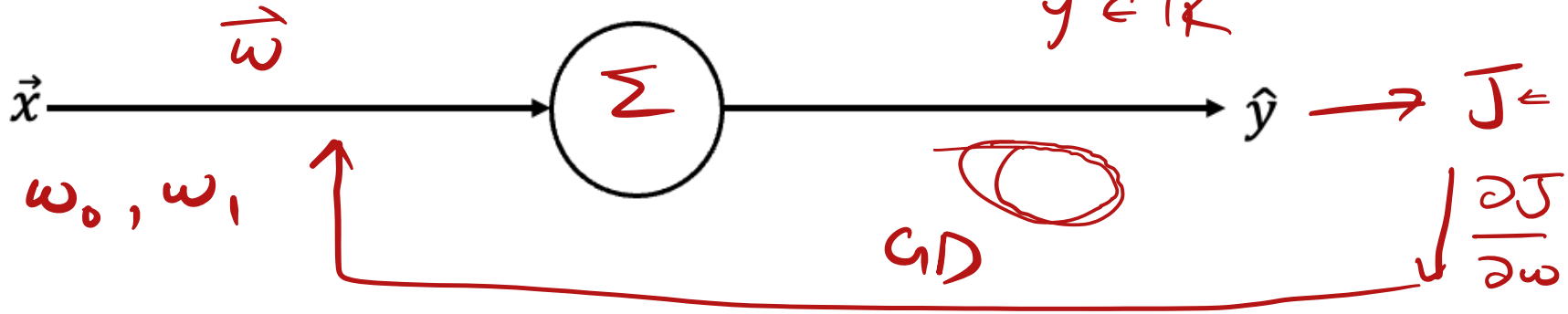
$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$x_0 = 1$

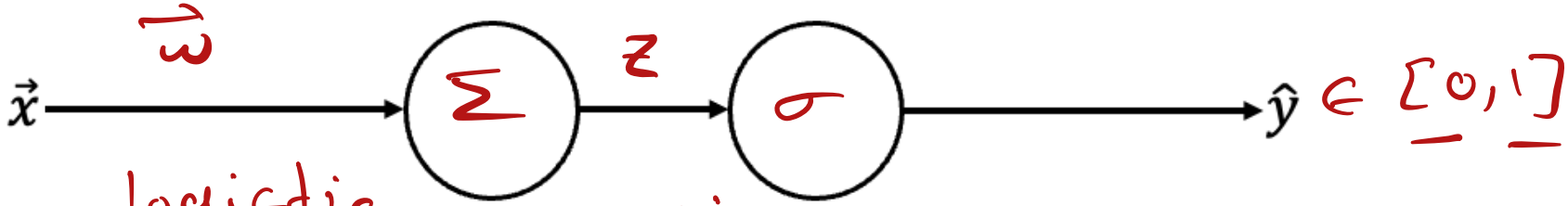
$y \to$ targets

$\hat{y} \to$ predictions

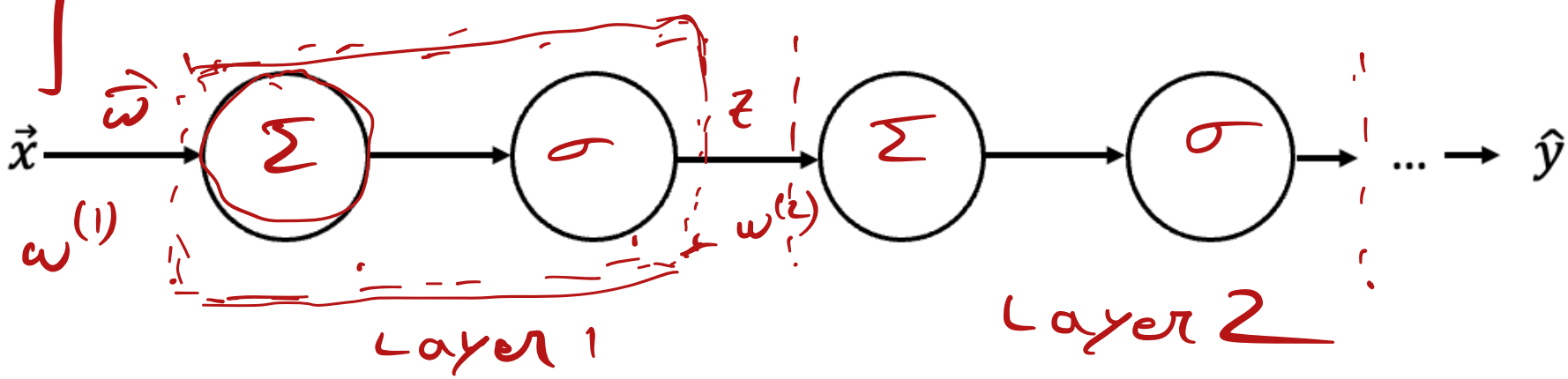
$\hat{y} \in \mathbb{R}$

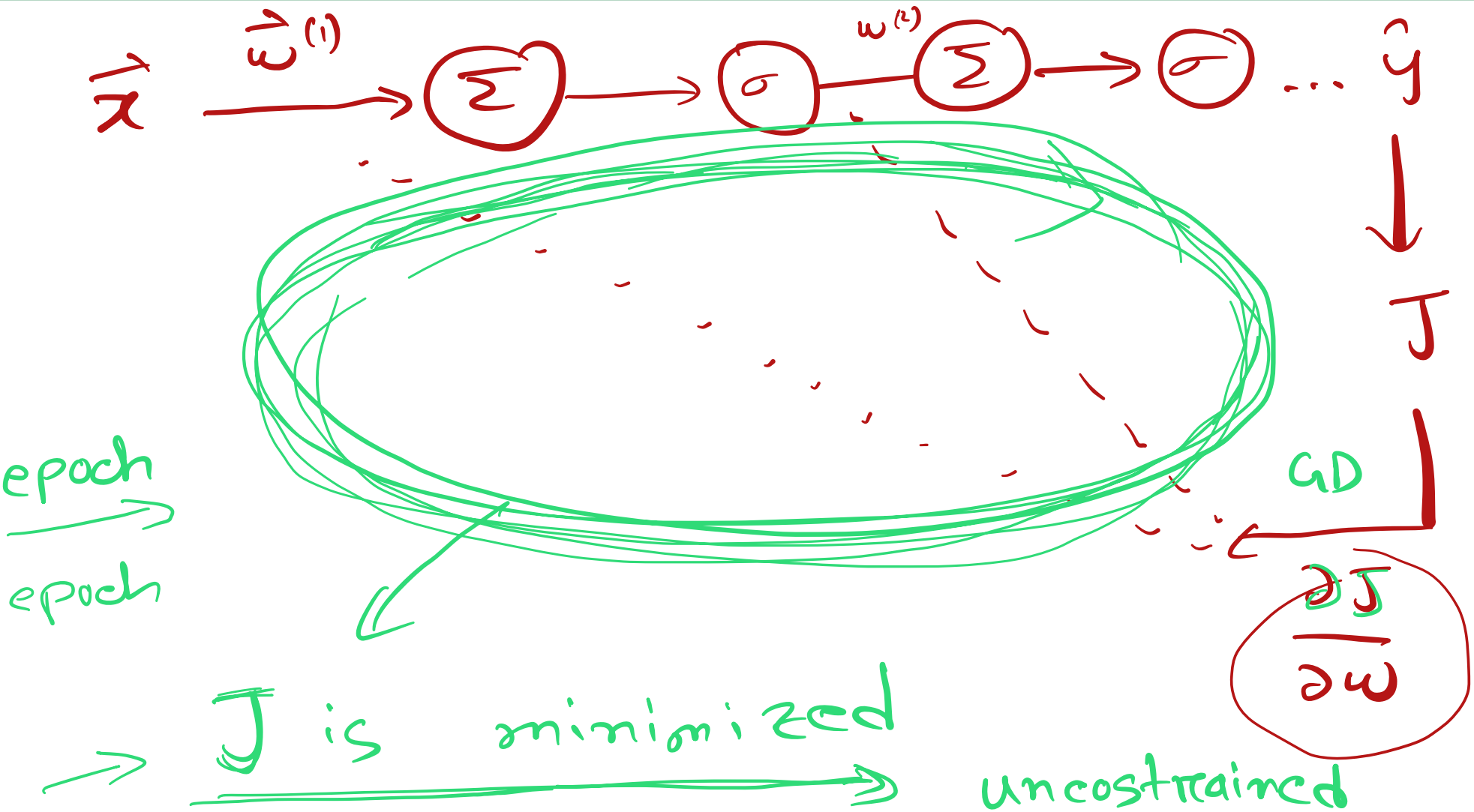


$$\begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$



logistic regression



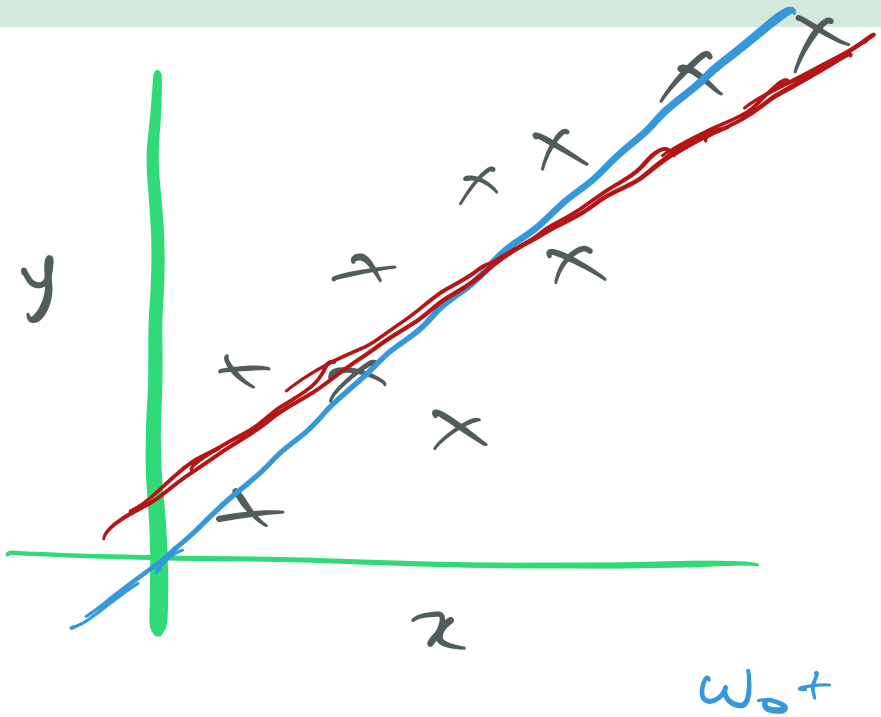

$\vec{x}$
$\vec{w}^{(1)}$
Σ
σ
$w^{(2)}$
Σ
σ
... $\hat{y}$
J
GD
$\frac{\partial J}{\partial w}$
epoch
epoch
J is minimized
unconstrained

Linear Hypothesis

Consider, m data points in the table,

predict y from a single input feature x

input	target	prediction
x_1	y_1	$\hat{y}_1$
x_2	y_2	$\hat{y}_2$
$\vdots$	$\vdots$	$\vdots$
x_m	y_m	$\hat{y}_m$



- we want to approximate target function $y = f(\underline{x}) = f(x_1, x_2, \ldots, x_n)$
- $\hat{y} = h(\underline{x}; \underline{w}) = w_0 + w_1 x_1$ [for $n = 1$, single feature, we have one input variable]
- x_1 is the input variable/feature not the data point in the equation.
- w's are called model parameters (weights), n is the number of feature
- Model parameters and hyperparameters are not same.
- Model parameters depend on training data, hyperparameters are chosen, or set, or optimized.

Cost function

How to train a linear model?

→ estimate mistakes and correct them via error measure.

It measures the total amount of incorrect predictions across the data points.

- squared error (loss), $\mathrm{L} = (y - \hat{y})^2$
- mean squared error, $mse = \frac{1}{m}\sum_i (y_i - \hat{y}_i)^2$
- cost function, $J = \frac{1}{2m}\sum_i (y_i - \hat{y}_i)^2$

m = no. of data

Gradient Descent to Minimize J

x_i y_i

$$J = \frac{1}{2m}\sum_i (y_i - w_0 - w_1 x_i)^2$$

$$\implies \frac{\partial J}{\partial w_0} = \frac{1}{2m}\sum_i \frac{\partial}{\partial w_0}(y_i - w_0 - w_1 x_i)^2$$

$$\frac{d}{dx}(x^n) = nx^{n-1}$$

$$\implies \frac{\partial J}{\partial w_0} = \frac{1}{2m}\sum_i \{2(y_i - w_0 - w_1 x_i)(0 - 1 - 0)\}$$

$$\implies \frac{\partial J}{\partial w_0} = -\frac{1}{m}\sum_i \{y_i - (w_0 + w_1 x_i)\}$$

$$\implies \frac{\partial J}{\partial w_0} = -\frac{1}{m}\sum_i (y_i - \hat{y}_i)$$

$$\therefore \frac{\partial J}{\partial w_0} = -\frac{1}{m}\sum_i (y_i - \hat{y}_i) = -\text{ average error}$$

Gradient Descent to Minimize J

$$J = \frac{1}{2m}\sum_i (y_i - w_0 - w_1 x_i)^2$$

$$\implies \frac{\partial J}{\partial w_1} = \frac{1}{2m}\sum_i \frac{\partial}{\partial w_1}(y_i - w_0 - w_1 x_i)^2$$

$$\implies \frac{\partial J}{\partial w_1} = \frac{1}{2m}\sum_i \{2(y_i - w_0 - w_1 x_i)\dot{(}0 - 0 - x_i)\}$$

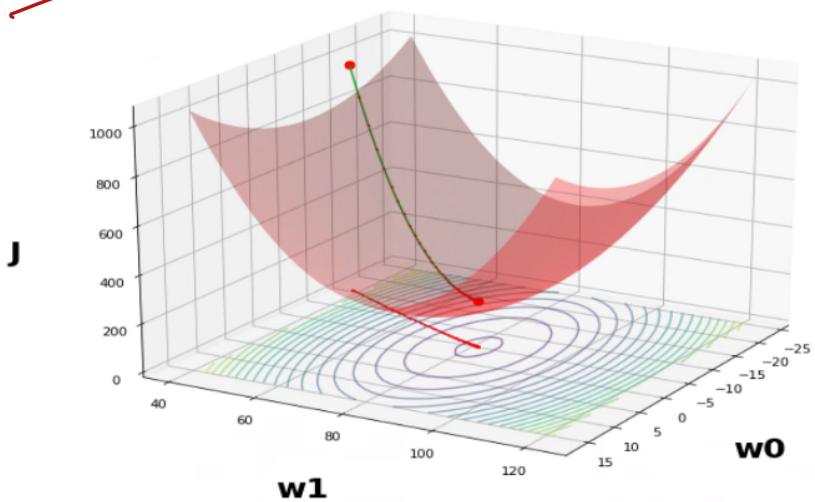
$$\implies \frac{\partial J}{\partial w_1} = -\frac{1}{m}\sum_i \{y_i - (w_0 + w_1 x_i)\}x_i$$

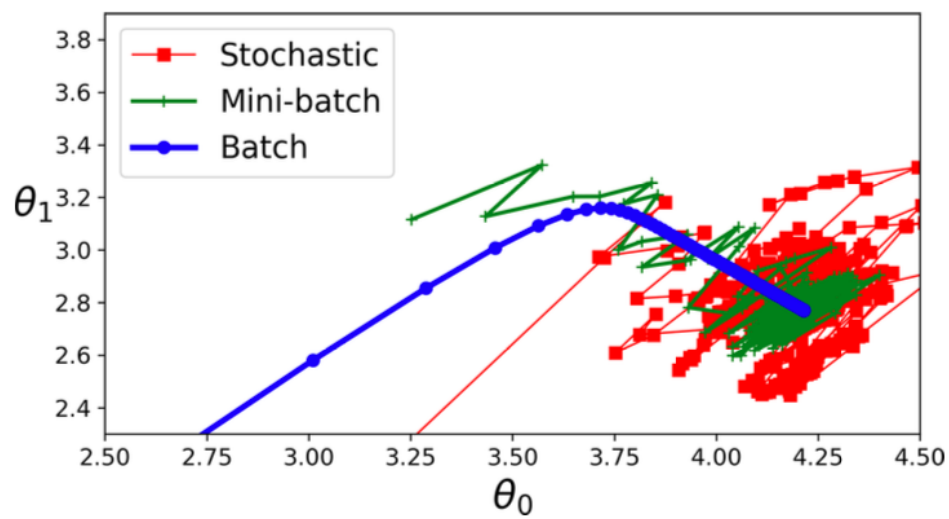
$$\implies \frac{\partial J}{\partial w_1} = -\frac{1}{m}\sum_i (y_i - \hat{y}_i)x_i$$

$$\therefore \frac{\partial J}{\partial w_1} = -\frac{1}{m}\sum_i (y_i - \hat{y}_i)x_i = -\text{ average error} \times \text{input}$$

Comparison of Gradient Descent Methods

- $w_{j+1} = w_j - \alpha \frac{\partial J}{\partial w_j}$
- Full batch, mini-batch, stochastic (SGDRegressor in Scikit).
- Works very well with large number of features with scaling.
- BGD with good learning schedule vs SGD vs mBGD, which would be better?
- Alternatives: Momentum, NAG, AdaGrad, RMSProp, Adam, AdaMax, Nadam.





Logistic Regression

Consider, m data points.
Predict y from input variables or features x_1, x_2

example	input $\underline{x} = (x_1, x_2)$	output y	prediction $\hat{y}$
1	$x_1^{(1)}, x_2^{(1)}$	y_1 = 0 or 1	$\hat{y}_1 = [0, 1]$
2	$x_1^{(2)}, x_2^{(2)}$	y_2 = 0 or 1	$\hat{y}_2 = [0, 1]$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
m	$x_1^{(m)}, x_2^{(m)}$	y_m = 0 or 1	$\hat{y}_m = [0, 1]$

Acc. P, R, F1, ROC
↳ scikit

Logistic Regression

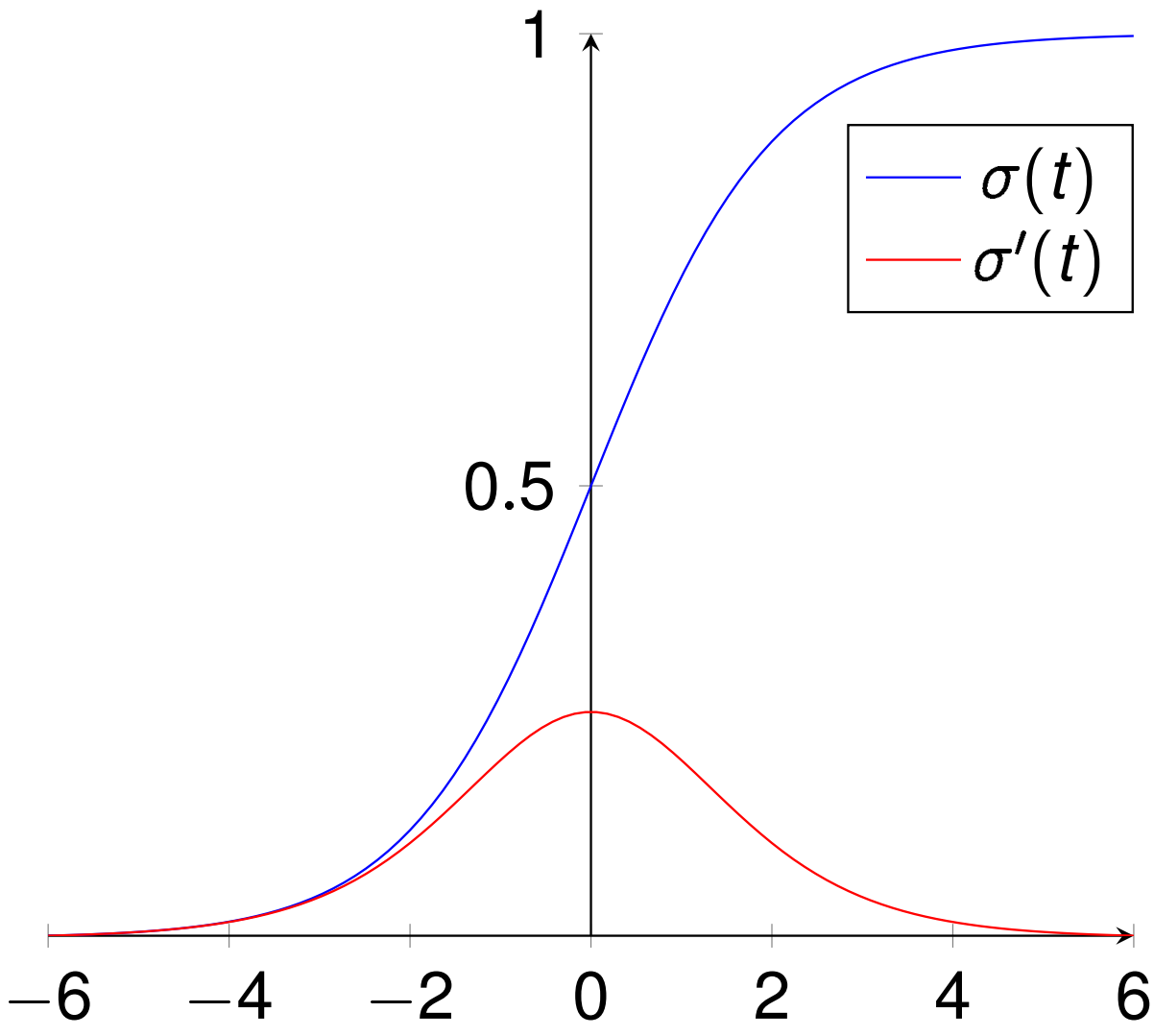
- $\hat{p} = h(\underline{x}; \underline{w}) = \sigma(w_0 + w_1 x_1 + w_2 x_2)$
- $z = w_0 + w_1 x_1 + w_2 x_2$
- $\sigma(t) = \frac{1}{1+e^{-t}}$
- $\hat{y} = \begin{cases} 0 & \text{if } \hat{p} < 0.5 \\ 1 & \text{if } \hat{p} \geq 0.5 \end{cases}$
- It handles extreme feature values quite well.

0.001

0.999

Cost function:, $J = -\frac{1}{m} \sum_i [y_i ln\hat{y}_i + (1 - y_i) ln(1 - \hat{y}_i)]$

Sigmoid function



$\sigma'(t) = \sigma(t)[1 - \sigma(t)]$ [Check it]

Cost function

How to train a logistic model for classification?

$\rightarrow$ "Squish" outputs between 0 and 1

$\rightarrow$ Binary classification

Least squares, absolute, and/or squared error are not good cost functions for classification because they do not penalize the model enough.

- cost function, $J = -\frac{1}{m}\sum_i [y_i ln\hat{y}_i + (1 - y_i) ln(1 - \hat{y}_i)]$
- If $y_i = \hat{y}_i$, for all data points then $J = 0$.
- If $y_i \neq \hat{y}_i$, for some data points then $J \rightarrow \infty$
- J should be positive, differentiable, and continuous.

Outputs of this cost function

Let's consider a single data point,

- $J = -[y ln\hat{y} + (1-y) ln(1-\hat{y})]$

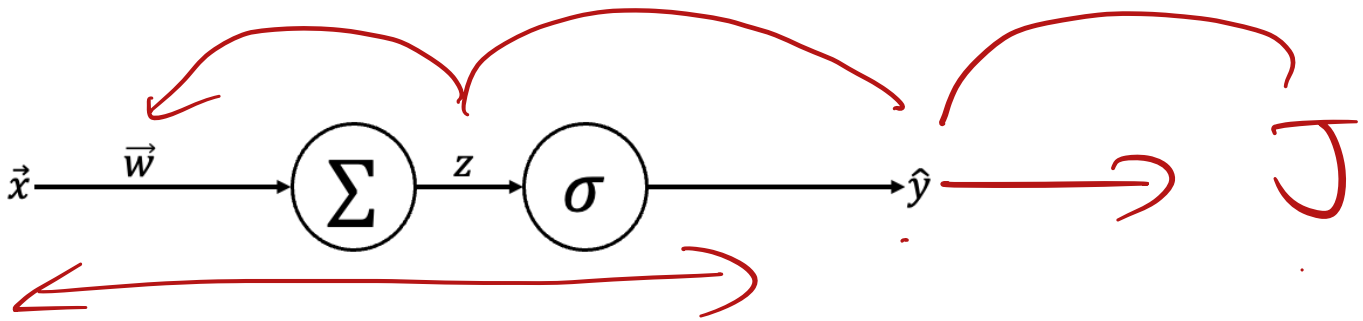
Correct classification

- $J \approx 0$, when $y = 0$ and prediction is $\hat{y} \approx 0$
- $J \approx 0$, when $y = 1$ and prediction is $\hat{y} \approx 1$

Incorrect classification

- $J \to \infty$, when $y = 0$ and prediction is $\hat{y} \approx 1$
- $J \to \infty$, when $y = 1$ and prediction is $\hat{y} \approx 0$

Derivative of log-loss cost function

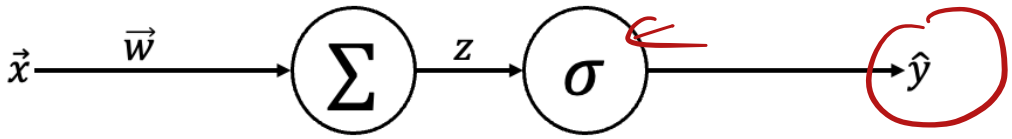


$$\frac{\partial J}{\partial w} = ?$$

$$\frac{\partial J}{\partial w} = \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} \frac{\partial z}{\partial w}$$

Chain Rule

$$\frac{d}{dx} f(g(x)) = f'(g(x)) \cdot g'(x)$$



Consider, the binary cross-entropy loss for a single data point,

$$J = -[y ln\hat{y} + (1-y)ln(1-\hat{y})]$$

$$\frac{d}{dx} \ln x = \frac{1}{x}$$

$$\implies \frac{\partial J}{\partial \hat{y}} = -[\frac{y}{\hat{y}} - \frac{1-y}{1-\hat{y}}]$$

$$\hat{y} = \sigma(z)$$

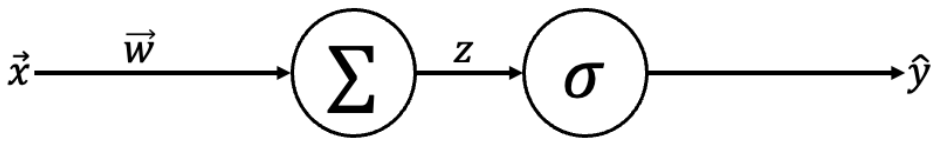
$$\frac{\partial \hat{y}}{\partial z} = \frac{\partial \sigma(z)}{\partial z}$$

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

$$\implies \frac{\partial \hat{y}}{\partial z} = \sigma'(z)$$

$$\implies \frac{\partial \hat{y}}{\partial z} = \sigma(z)[(1-\sigma(z))]$$

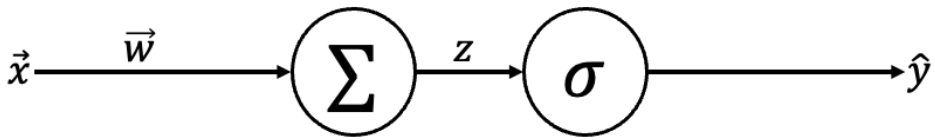
$$\implies \frac{\partial \hat{y}}{\partial z} = \hat{y}(1-\hat{y})$$



$$\frac{\partial J}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial z} = -[\frac{y}{\hat{y}} - \frac{1-y}{1-\hat{y}}]\hat{y}(1-\hat{y})$$

$$\frac{\partial J}{\partial z} = -(\frac{y - \cancel{y\hat{y}} - \hat{y} + \cancel{y\hat{y}}}{\hat{y}(1-\hat{y})})\hat{y}(1-\hat{y})$$

$$\frac{\partial J}{\partial z} = -(y - \hat{y}) = -\textbf{error}$$



$$\frac{\partial z}{\partial w_1} = \frac{\partial}{\partial w_1}(w_0 + w_1 x_1) = x_1 = \textbf{input} \quad \text{[single feature]}$$

We can check the above for more than one features and write generally as

$$\frac{\partial J}{\partial w} = \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} \frac{\partial z}{\partial w} = -(y - \hat{y})x = \textbf{error} \times \textbf{input}$$

Considering m data points we obtain,

$$\frac{\partial J}{\partial w_j} = -\frac{1}{m} \sum_{i=1}^{m} (y_i - \hat{y}_i) x_j$$

Scikit

'L2'

LRC-model

GD

LRC

OR Gate and NOR Gate

input $\underline{x} = (x_1, x_2)$	output y	prediction
(0,0)	0	< 0.5
(0,1)	1	≥ 0.5
(1,0)	1	≥ 0.5
(1,1)	1	≥ 0.5

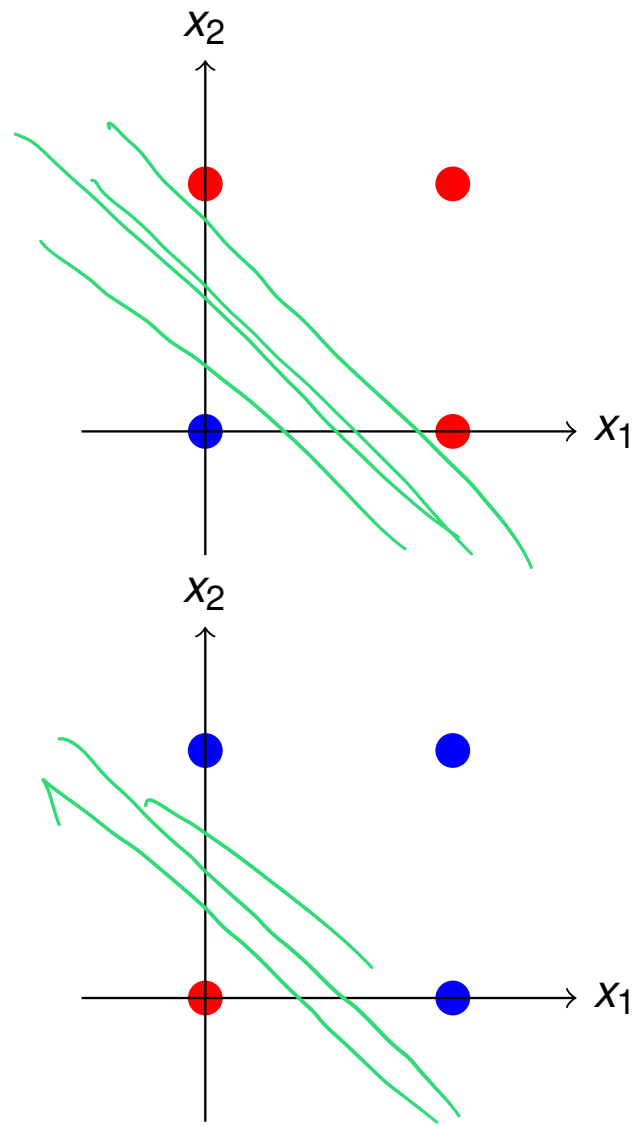
OR Gate: $w_0 = -1$ $w_1 = 2$ $w_2 = 2$

input $\underline{x} = (x_1, x_2)$	output y	prediction
(0,0)	1	≥ 0.5
(0,1)	0	< 0.5
(1,0)	0	< 0.5
(1,1)	0	< 0.5

NOR Gate: $w_0 = 1$ $w_1 = -2$ $w_2 = -2$

Note: w's are not guaranteed to be unique

red-1, blue-0



AND Gate and NAND Gate

input $\underline{x} = (x_1, x_2)$	output y	prediction
(0,0)	0	< 0.5
(0,1)	0	< 0.5
(1,0)	0	< 0.5
(1,1)	1	≥ 0.5

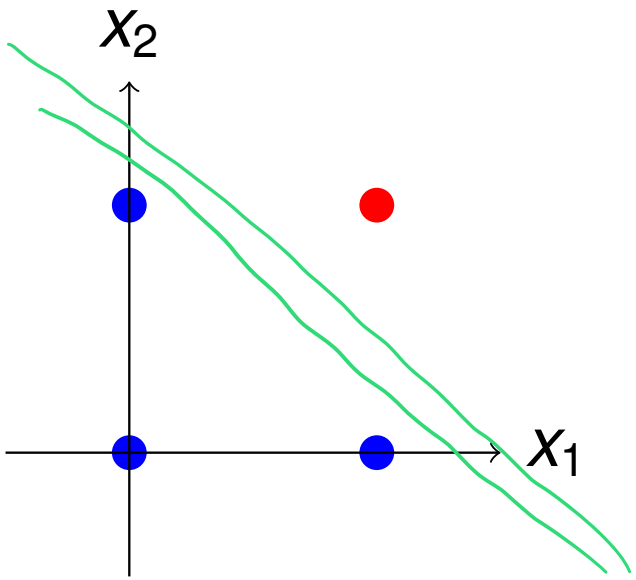
AND Gate: $w_0 = -3$ $w_1 = 2$ $w_2 = 2$

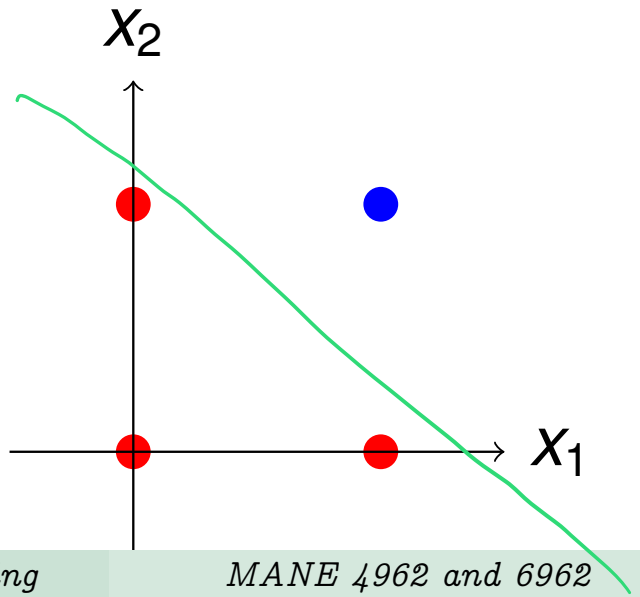
input $\underline{x} = (x_1, x_2)$	output y	prediction
(0,0)	1	≥ 0.5
(0,1)	1	< 0.5
(1,0)	1	< 0.5
(1,1)	0	< 0.5

NAND Gate: $w_0 = 3$ $w_1 = -2$ $w_2 = -2$

Note: w's are not guaranteed to be unique

red-1, blue-0





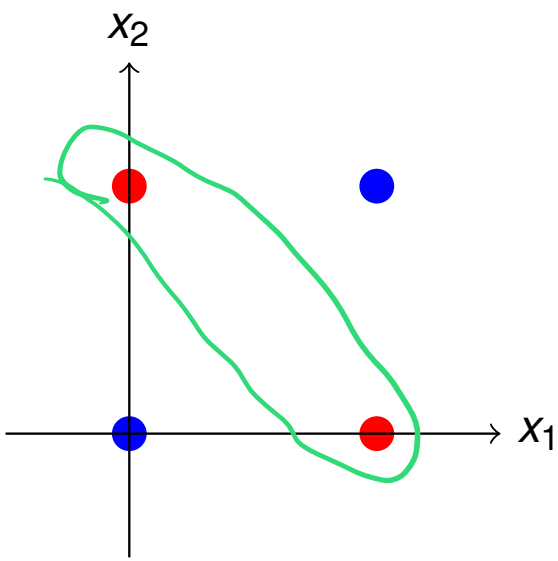
XOR Gate

input $\underline{x} = (x_1, x_2)$	output y	prediction
(0,0)	0	×
(0,1)	1	×
(1,0)	1	×
(1,1)	0	×

XOR Gate: No solution from logistic regression!

- Use non-linear feature transformation. (The kernel trick) SVMs.
- Add extra layers. (Deep neural nets)

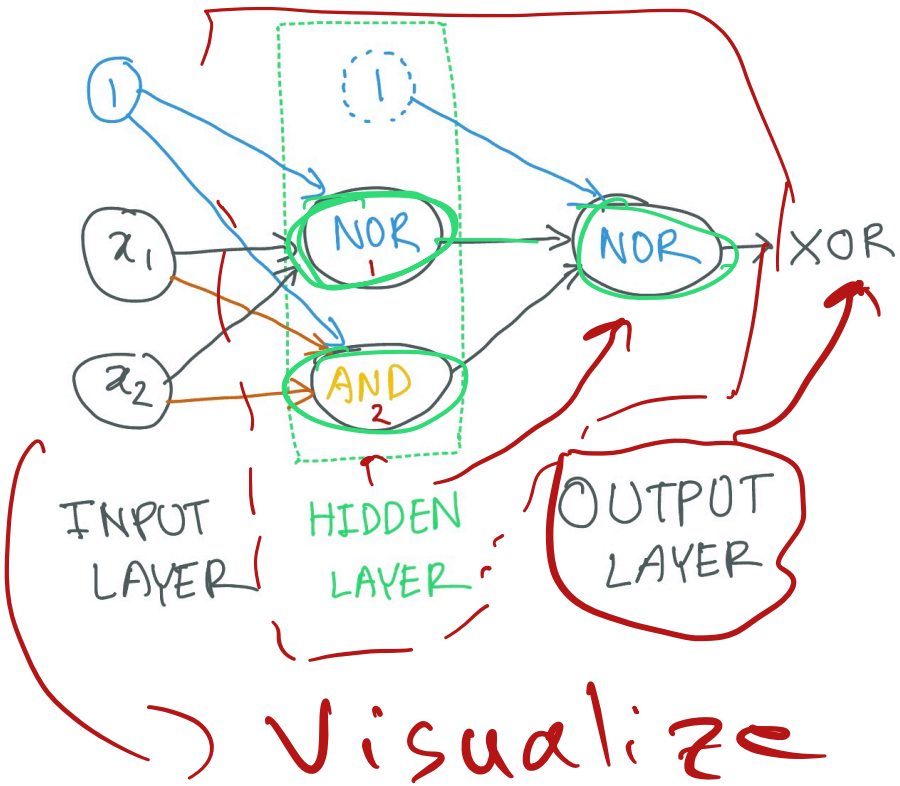
red-1, blue-0



Not linearly separable

Solving XOR Gate

Let's consider,



Visualize

$\underline{x}$ (x_1, x_2)	(h_1, h_2) = (NOR, AND)	NOR(h_1, h_2) = XOR
(0,0)	1, 0	0
(1,0)	0, 0	1
(0,1)	0, 0	1
(1,1)	0, 1	0

First NOR: $w_{01}^{(1)} = 1$ $w_{11}^{(1)} = -2$ $w_{21}^{(1)} = -2$

AND Gate: $w_{02}^{(1)} = -3$ $w_{12}^{(1)} = 2$ $w_{22}^{(1)} = 2$

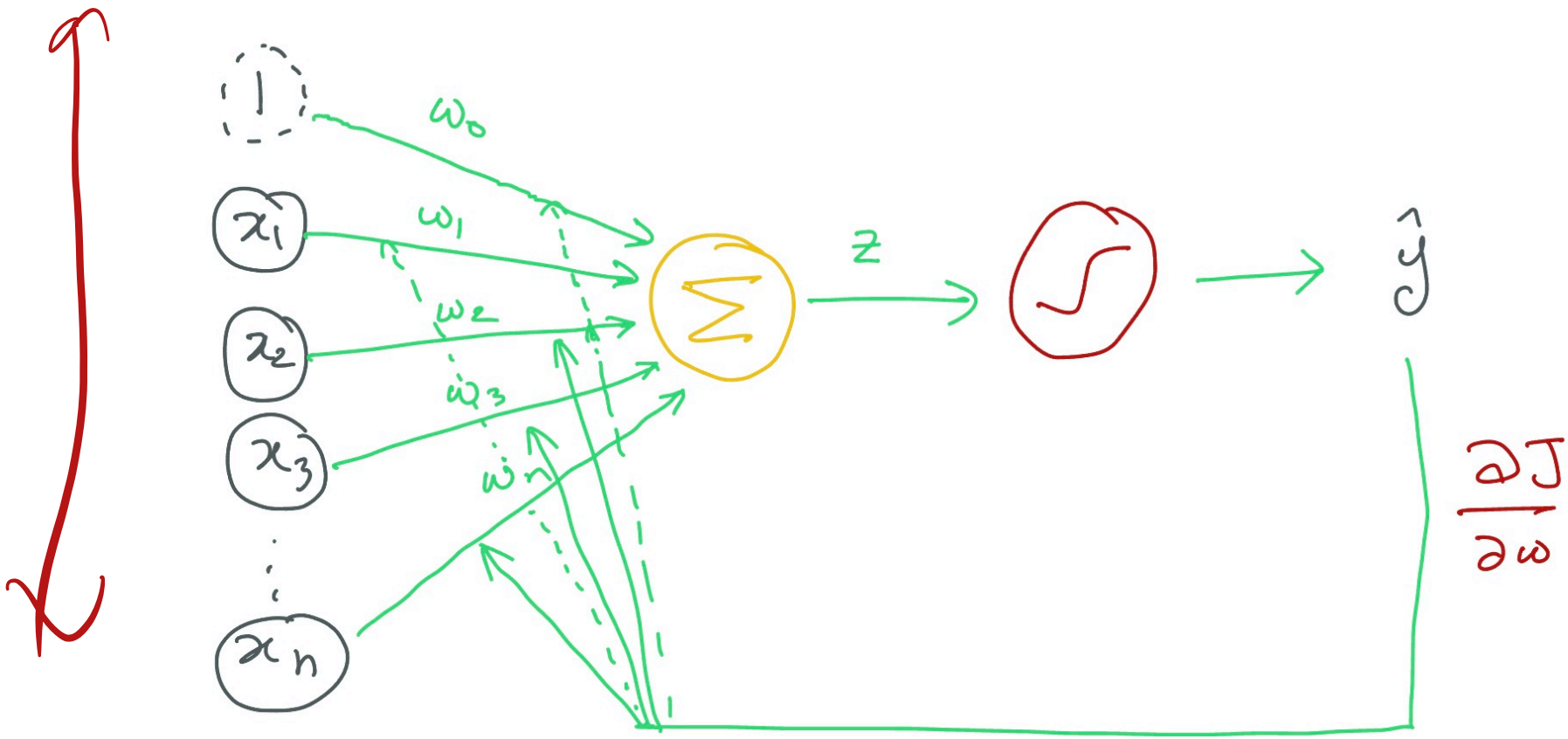
Last NOR : $w_{01}^{(2)} = 1$ $w_{11}^{(2)} = -2$ $w_{21}^{(2)} = -2$

HW4 P4

0 0 0

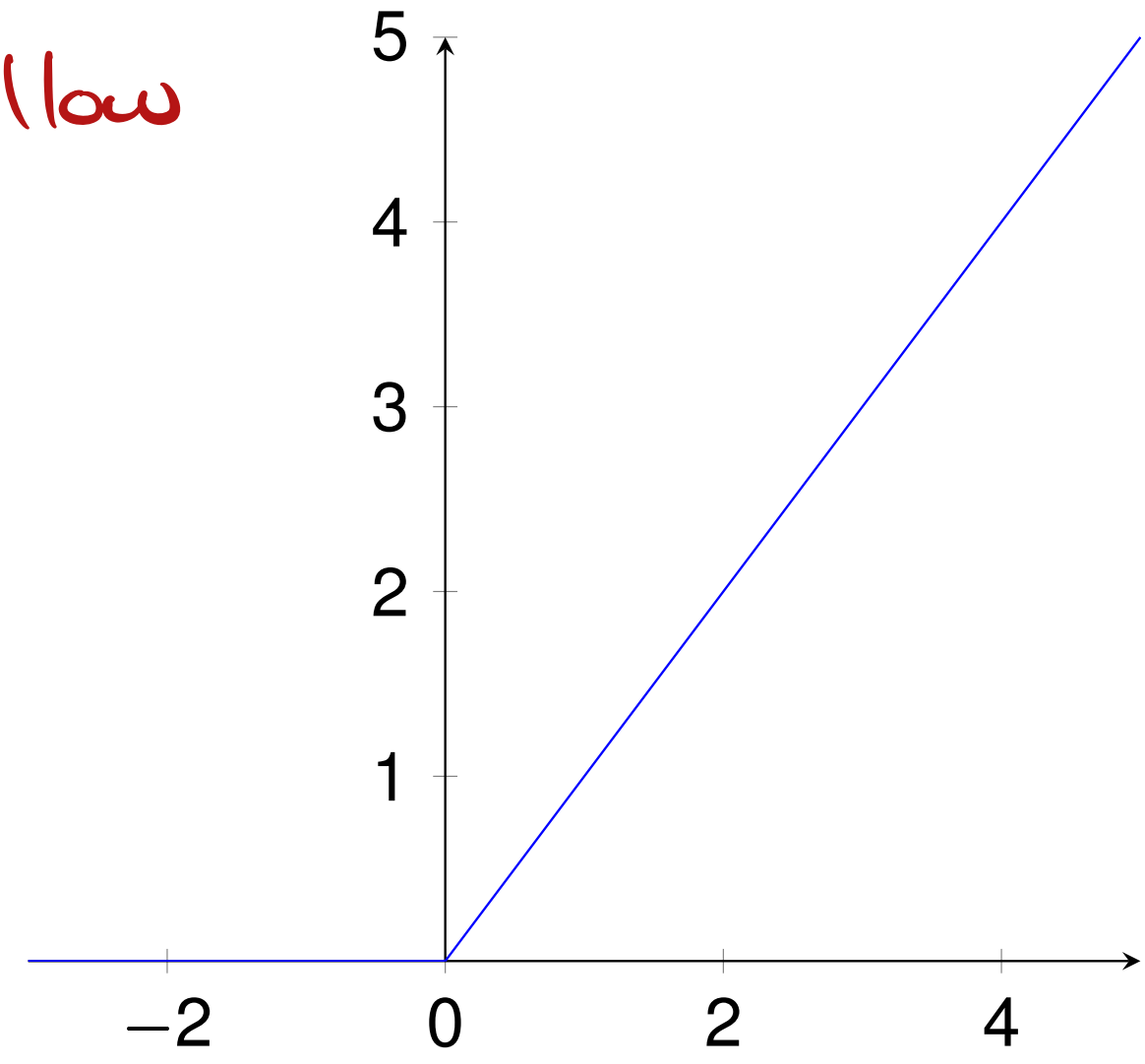
0

Moving beyond gates (More than 2 features)



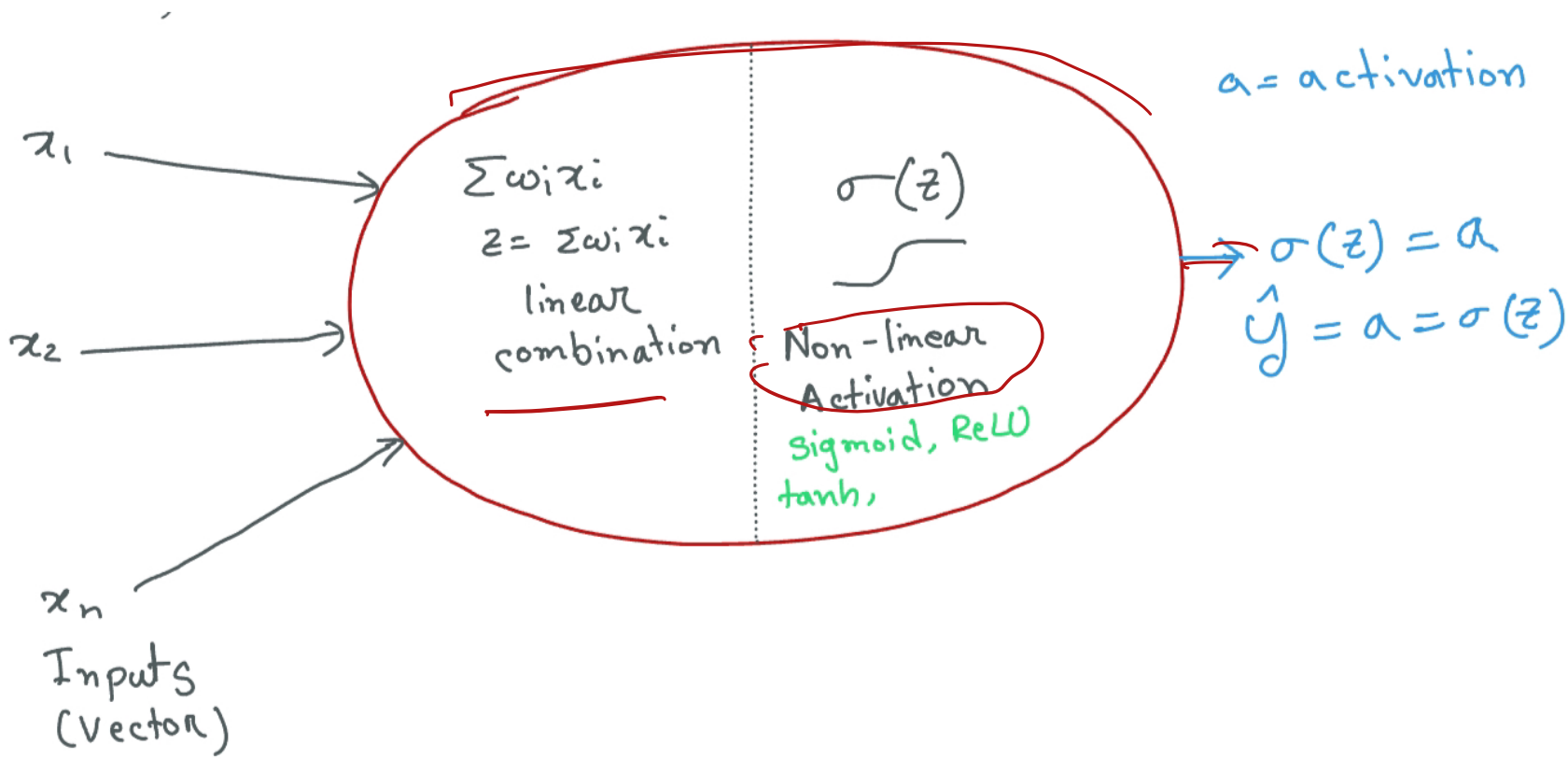
Rectified Linear Unit

Goodfellow

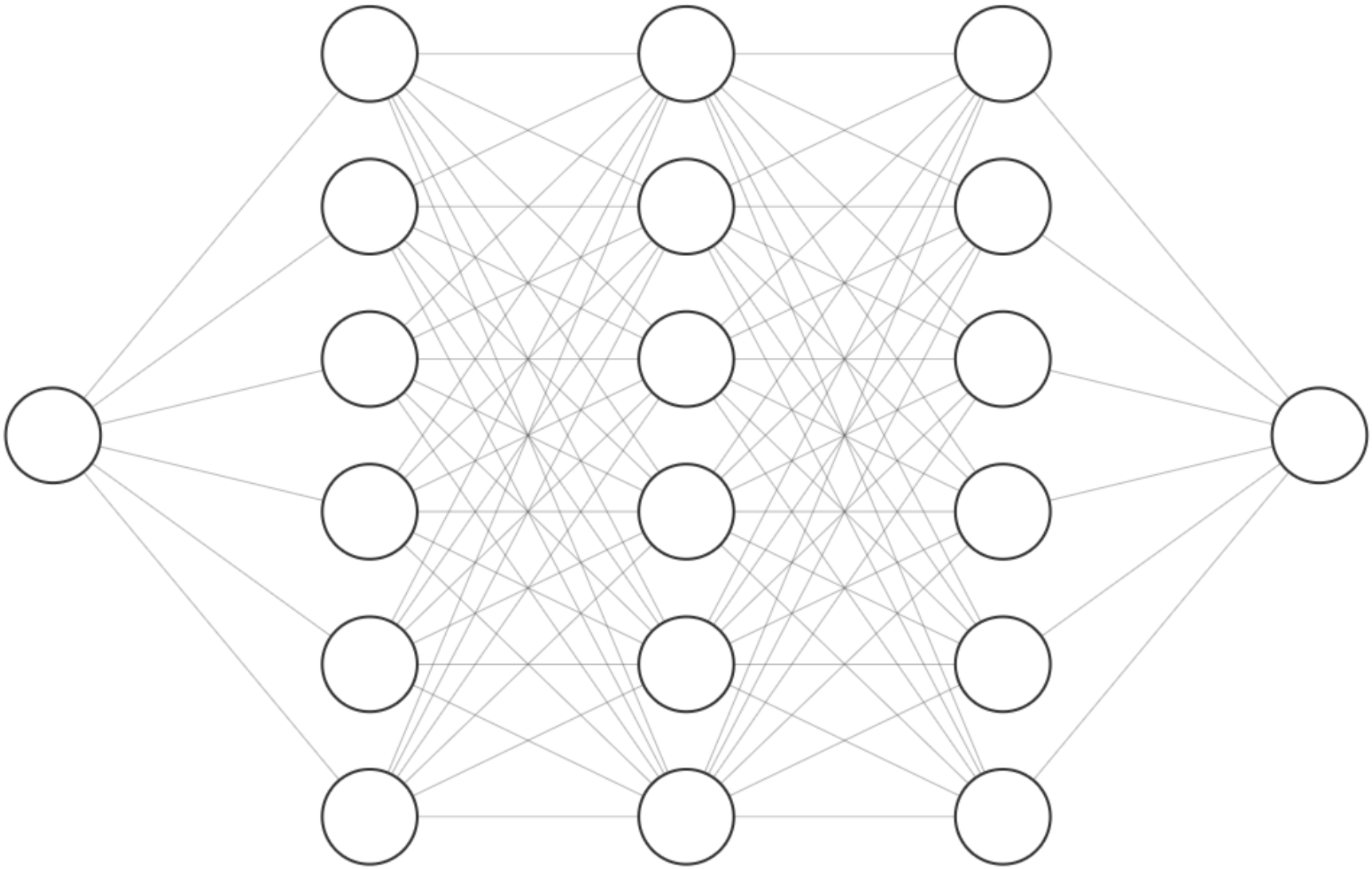


$ReLU(t) = max(0, t)$

Artificial Neuron



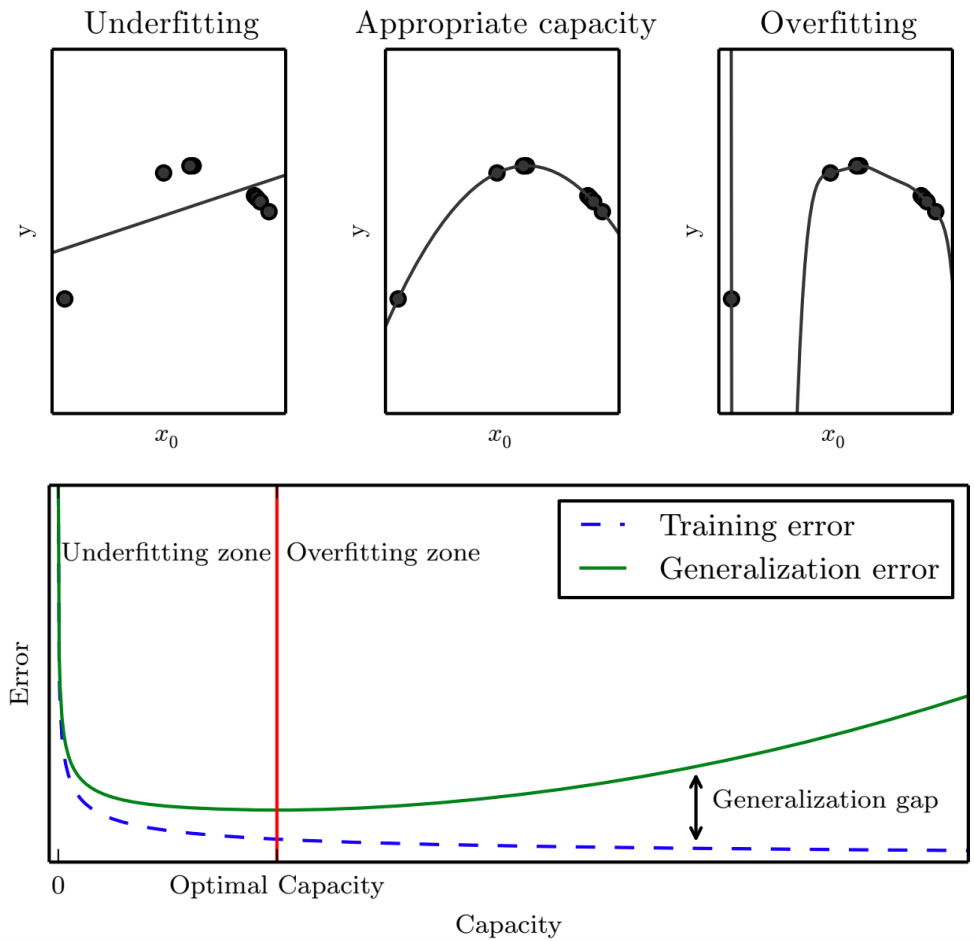
A fully connected deep ANN



A fully connected deep ANN

```
model = Sequential()
model.add(Dense(6, input_dim=1,
        activation='relu'))
model.add(Dense(6,activation='relu'))
model.add(Dense(6,activation='relu'))
model.add(Dense(1))
opt = optimizers.Adam(learning_rate=0.001)
mse = tf.keras.losses.MeanSquaredError(
    reduction=tf.keras.losses.Reduction.SUM)
model.compile(loss=mse, optimizer=opt)
model.fit(X,y,epochs=2000,batch_size=10, verbose=0)
predictions = model.predict(X)
```

Analyzing the learning process



Overfitting, underfitting, capacity, bias, and variance

Regularization

- To regularize a model, means to constrain it and not make it too complex.
- **Ridge:** Force model to choose smaller weights. $\lambda \sum |w_i|^2$ term is added to cost function. λ is the strength of regularization, a hyperparameter.

L2 Regularized

- **Lasso:** Make weights of less important features zero. $\lambda \sum |w_i|$.
- **ElasticNet:** $r\lambda \sum |w_i| + \frac{1-r}{2}\lambda \sum |w_i|^2$ term is added to cost function, r is the mix ratio.
- **Early stopping**: Stop training as soon as the validation error reaches a minimum.
- Scikit implements regularization for SGDRegressor, logistic regression and many other methods. Read the documentation carefully.

'L2'

SGDRegressor

(λ_1 =)

Testing and Validating

- Some data is kept away so the model can generalize on data it has never seen.
- multiple sets - commonly training data, testing data and validation data.
- Other splits performed for finding hyperparamters or stricter evaluation
- kfoldCV, RFECV, LOOCV etc.
- Hyperparameters are tuned with CV or eshtablished from heuristics and experience
- Changing a hyperparamter will yield a new model/hypothesis.

- **No Free Lunch Theorem:** If you make absolutely no assumption about the data, then there is no reason to prefer one model over any other. (Wolpert and Macready, 1996)
- No model is a priori guaranteed to work better.
- **Universal approximation theorem:** One hidden layer is enough to represent (not learn) an approximation of any function to an arbitrary degree of accuracy. (Goodfellow et al.)

Image → do not
70-30

Metrics: Evaluating ML models

Evaluate classifier

For classification

- Confusion matrix
- Classification accuracy (CA)
- Precision (P), Recall (R), F1 score
- Precision-recall curve
- Receiver operating characteristic (ROC) curve

Evaluate your estimator
Regressor

For regression

- Coefficient of determination
- MAE
- MSE
- Plots of actual vs predicted values, or residuals vs predicted values are also useful. The coefficient of determination is useful for linear regression.

For clustering

- Elbow plot
- Silhouette scores

Not really

How to prepare for the exam?

Python

- Study the notebooks from lectures 1,2,4,5, and 7.
- Understand the concepts and all the datasets from the lectures.
- Supervised models need annotated data, unsupervised models do not.
- Classification and regression are supervised learning methods.
- Practice preprocessing your data (odd and even), importing via pandas, Numpy etc.
- Practice programming each ML model you have learned so far.
- Read the questions carefully and try to understand which ML task you need to perform to solve the problem.
- Visualize the data. Write what you observed in the dataset. Does the data appear to be linear? Is it sinusoidal?
- What are the inputs and the outputs? Which model do you need? What would be the cost function?
- Is your model optimized to make a "correct" prediction? What are the hyperparameters?
- Do you need regularization? Is your model overfitting? Or is it underfitting?
- Are you using the right metrics to evaluate the model?

How to submit the exam?

Unlimited

- Review the submission requirements.
- The exam submission is similar but not the same as HW assignments.
- Like HW assignments you will submit a single PDF.
- But you will also submit a MS Word document file with your specific answers to each question.
- A PDF and a DOC file is needed for the evaluation of your exam.
- The PDF will have your code and its outputs.
- The DOC will have your answers. Add images, plots, equations, etc but no code in the DOC file. Only your answers, in your own words, to each question.
- Organize and present your code in a clean and coherent manner.
- Do not print 200 data points in your notebook or generate 784 pairplots.
- Highlight and explain your code in your own words using notebook cells when generating a PDF.
- Remember: Code is read 100 times more than it is written.
- **Make it easier on yourself by keeping your code organized.**
- Check that you have answered the questions that were actually asked during your final review before submission.

2. ii) 120,000

3.