- No groupwork today
- 40 min – Logistic Regression
- 10 min – Break
- 40 min – Regularization
- 20 min - Discussion

Logistic Regression

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Binary Classification

1(cat) vs 0 (non cat)

1(spam) vs 0 (non spam)

Dataset: Annie's Youtube history

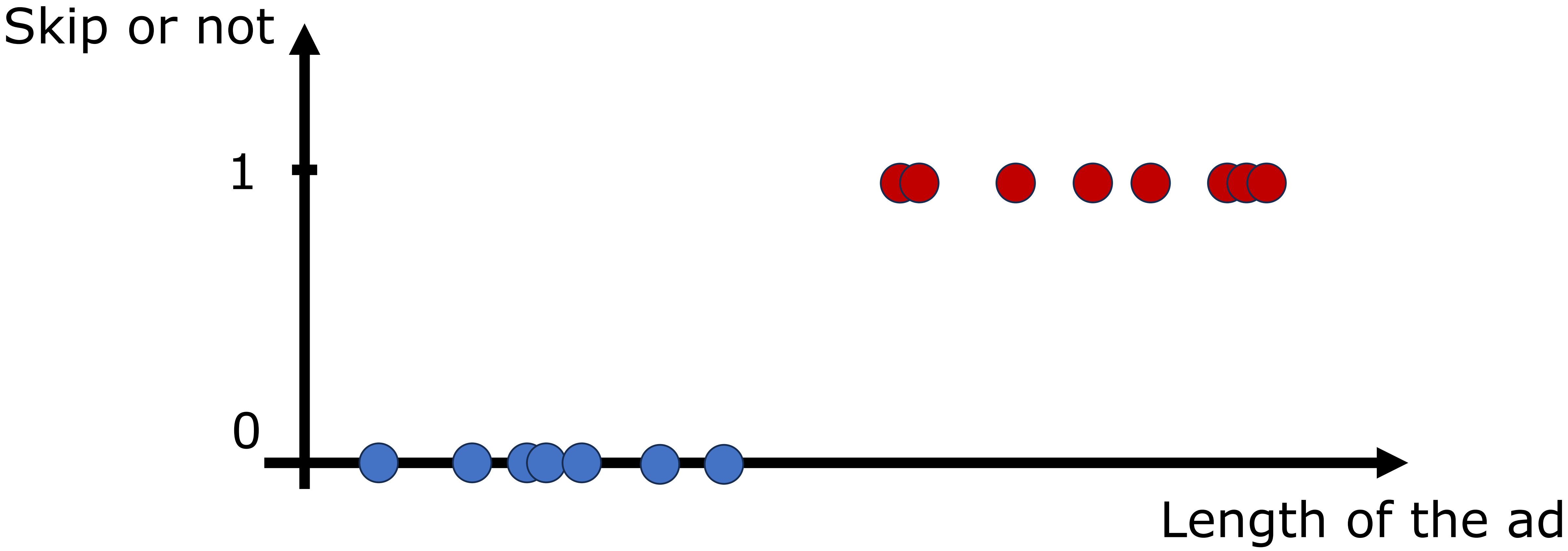
- Datapoints: $(x_i, y_i), \quad i = 1, 2, \ldots, n$
- x: the length of the advertisement
- y : whether Annie skips the advertisement

  $y = 1$ if Annie skips the ad;

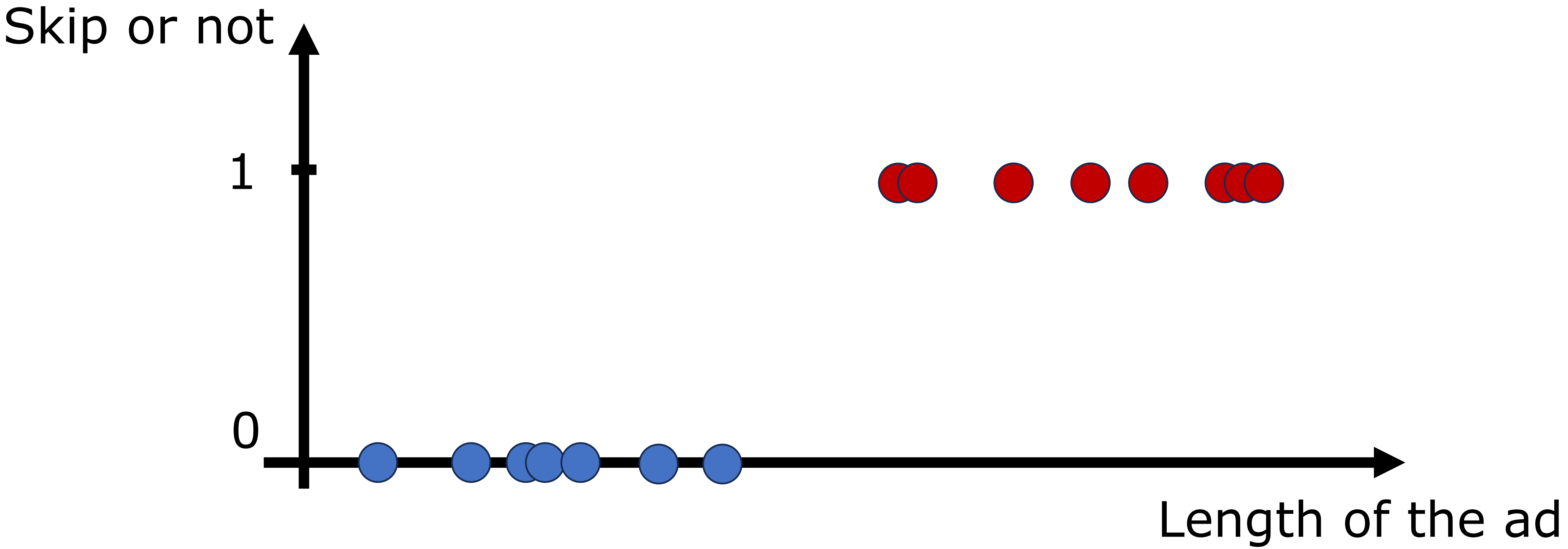
  $y = 0$ if Annie doesn't

- Goal: Given the length of an advertisement, predict whether Annie will skip it.

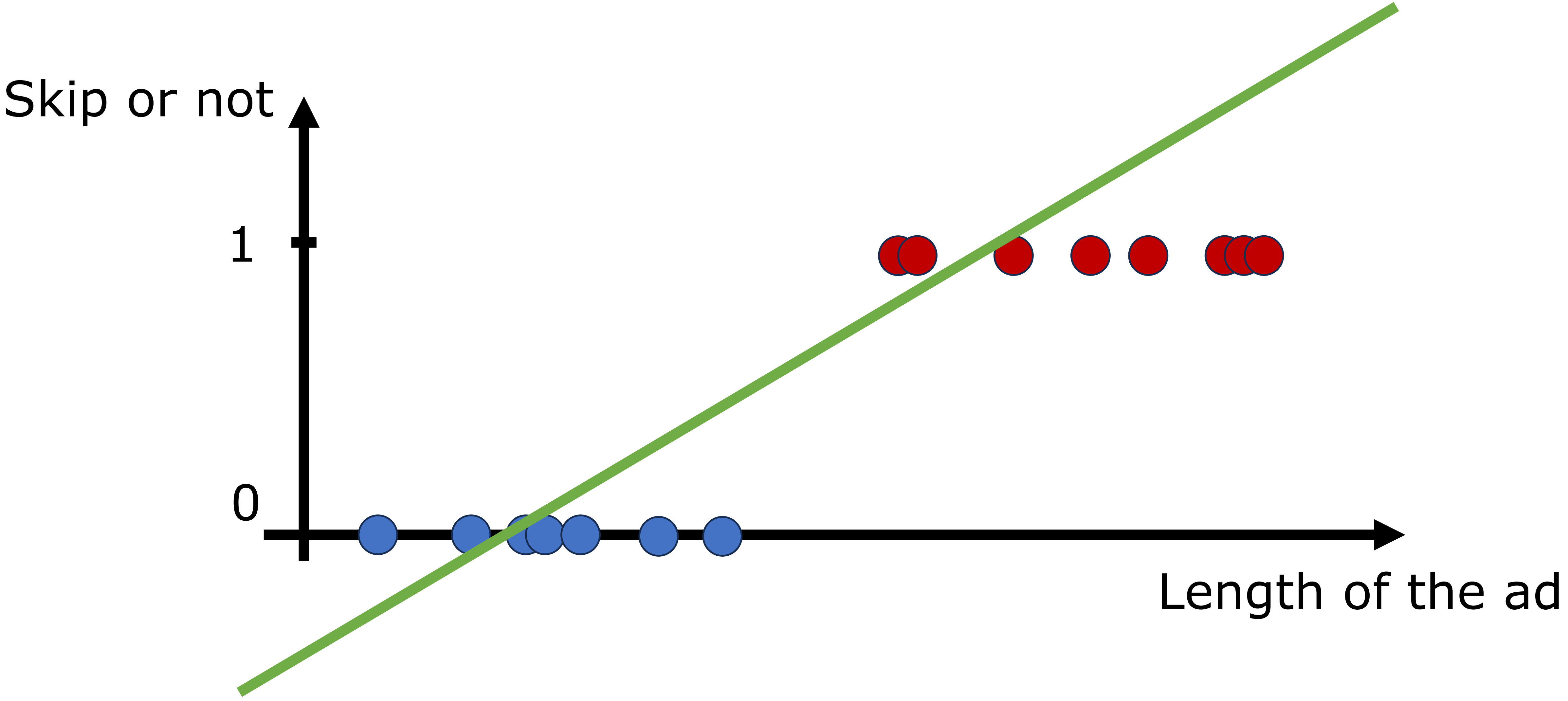
Visualize the datapoints



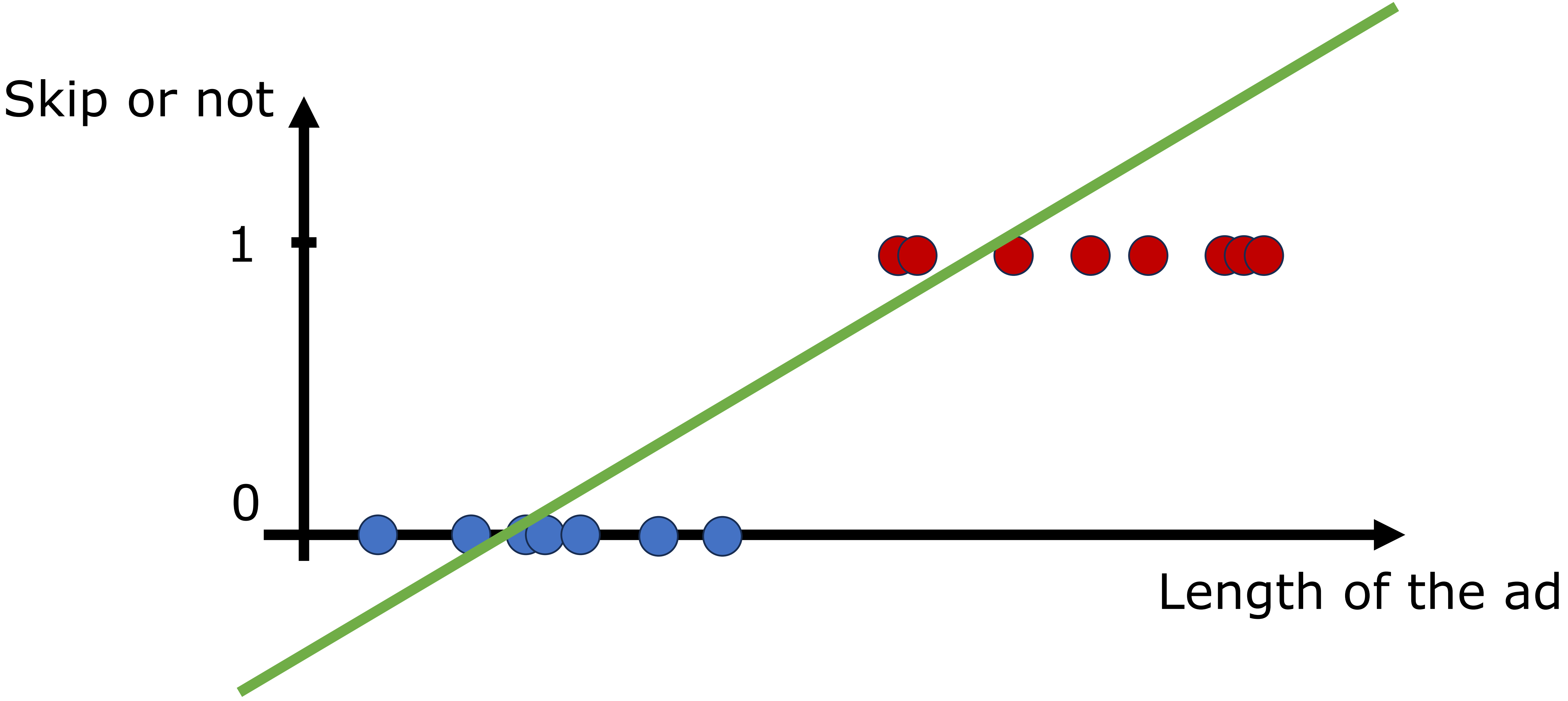
A function that fits the data?



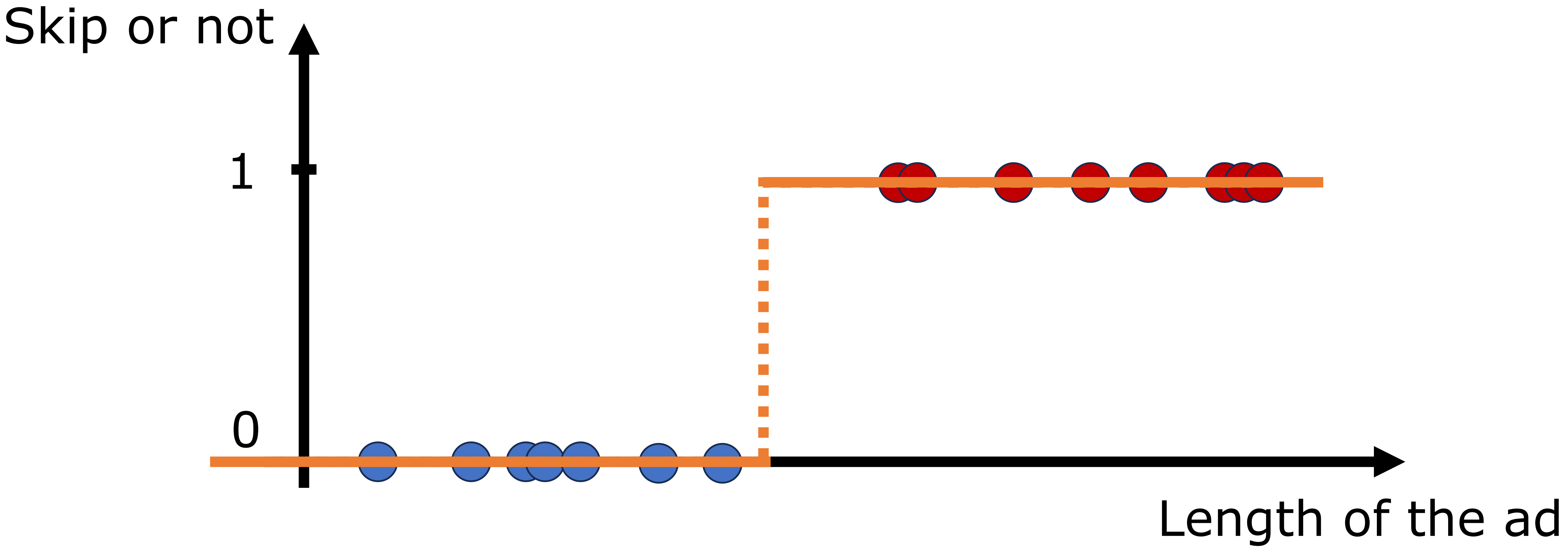
Linear Functions



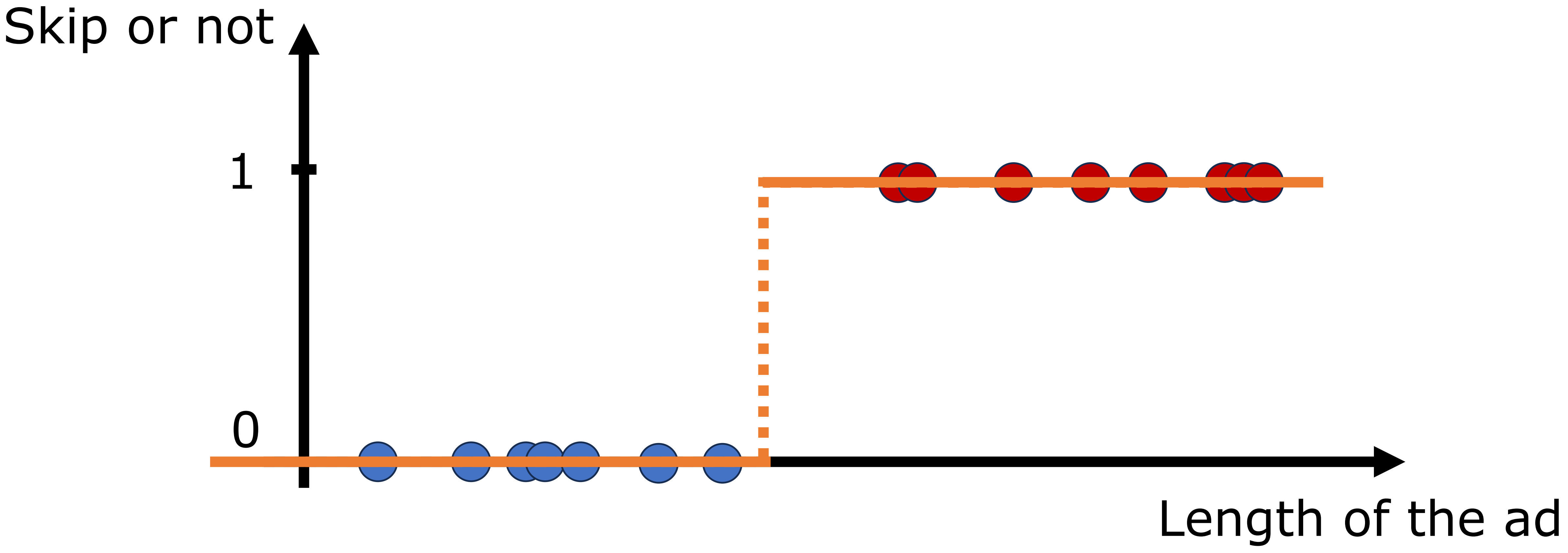
…too far away from the data



Step Functions

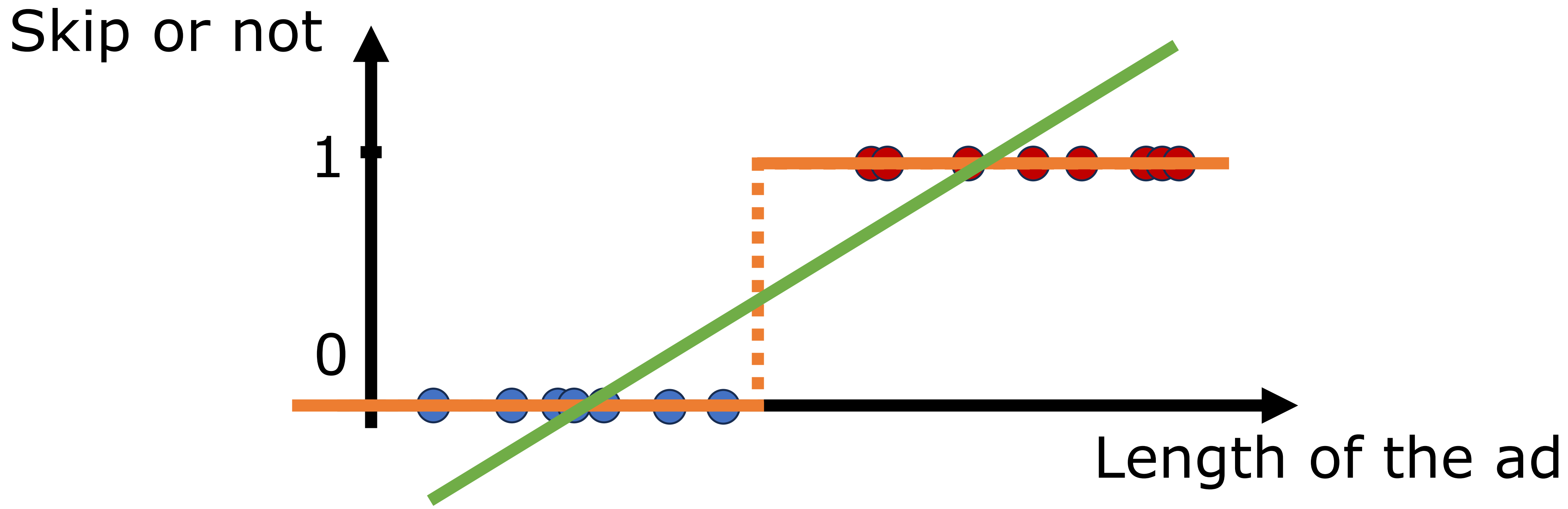


…not continuous



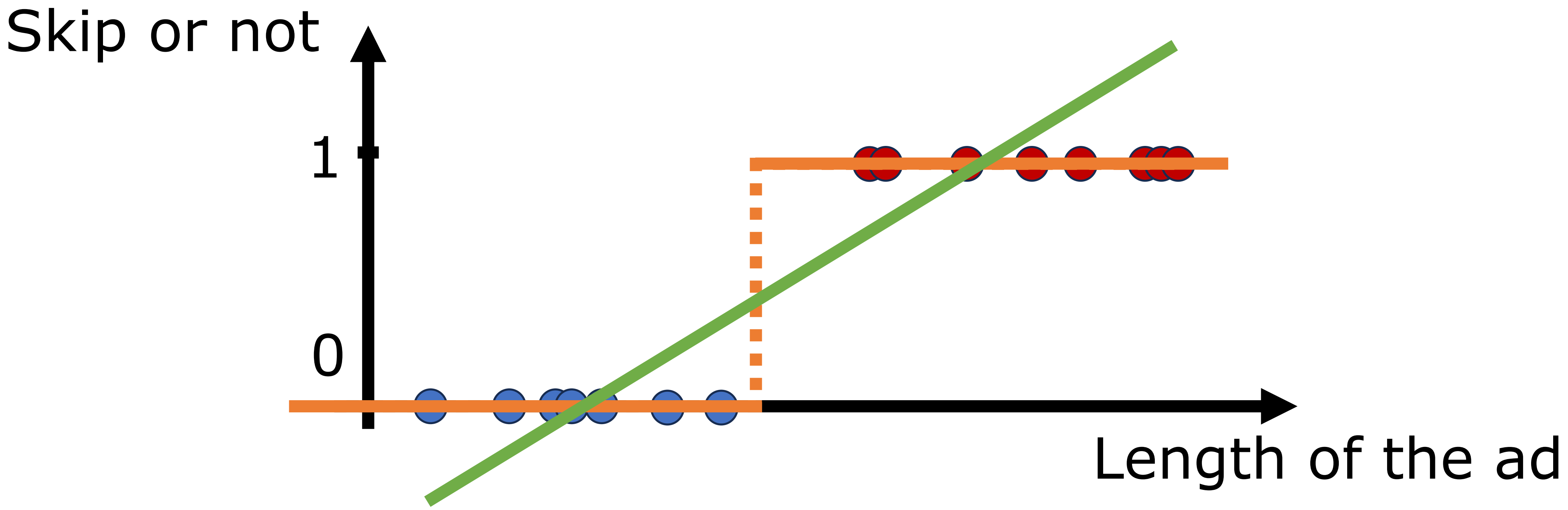
A good function class?

- 1. Close to the data
- 2. Continuous, tractable



A good function class?

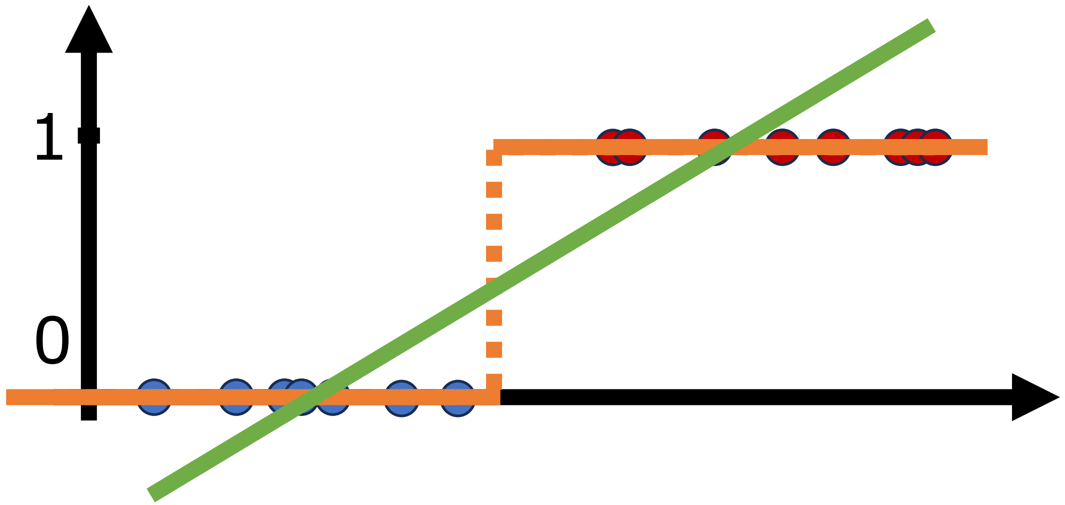
- 1. Close to the data – Step functions
- 2. Continuous, tractable – Linear functions



Can we combine them?

- "Compress"(or transform) the linear function into another continuous function that shapes like the step function.
- The range of linear functions is $[-\infty, \infty]$, but $y_i \in \{0, 1\}$.
- We want to find a function that maps

$$[-\infty, \infty] \rightarrow [0,1]$$

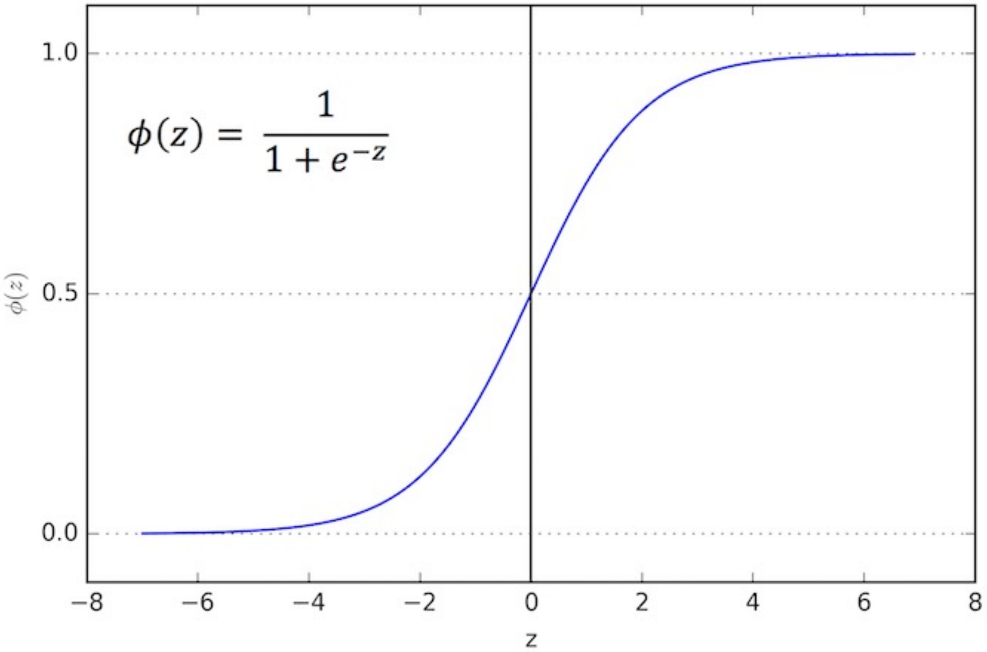


Logistic Function

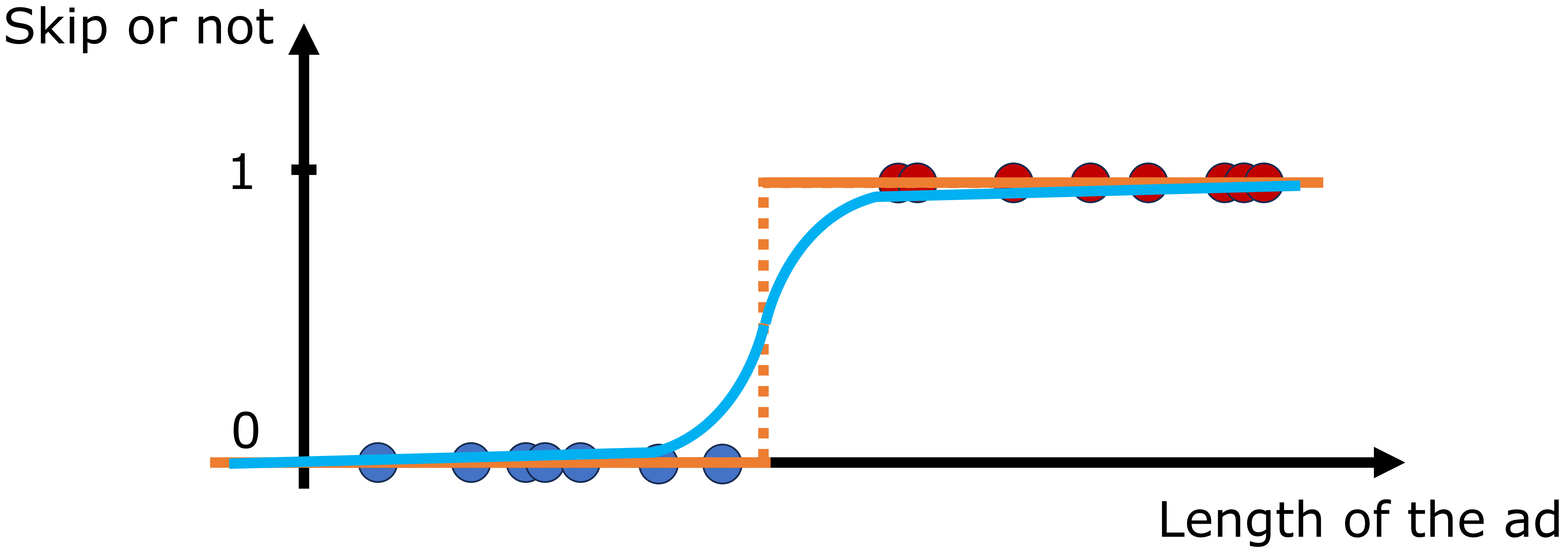
- A standard logistic function is an S-shaped curved

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

- $z \to \infty,\ \sigma \to \frac{1}{1+0} = 1$
- $z \to -\infty,\ \ \sigma \to \frac{1}{1+\infty} = 0$
- $z = 0,\ \sigma = \frac{1}{2}$



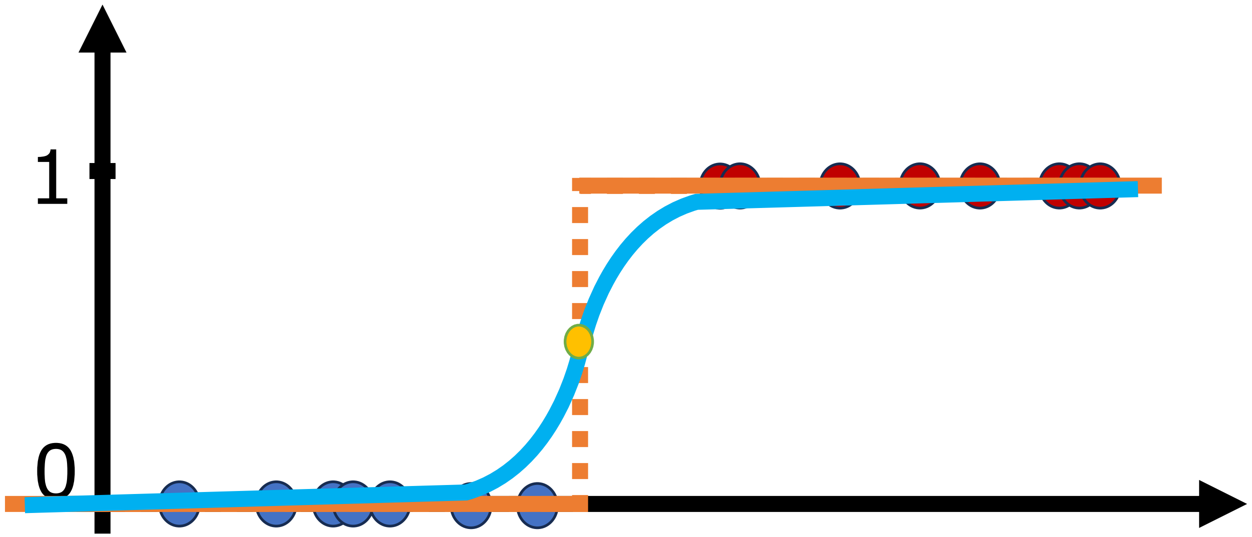
Smooth the step function



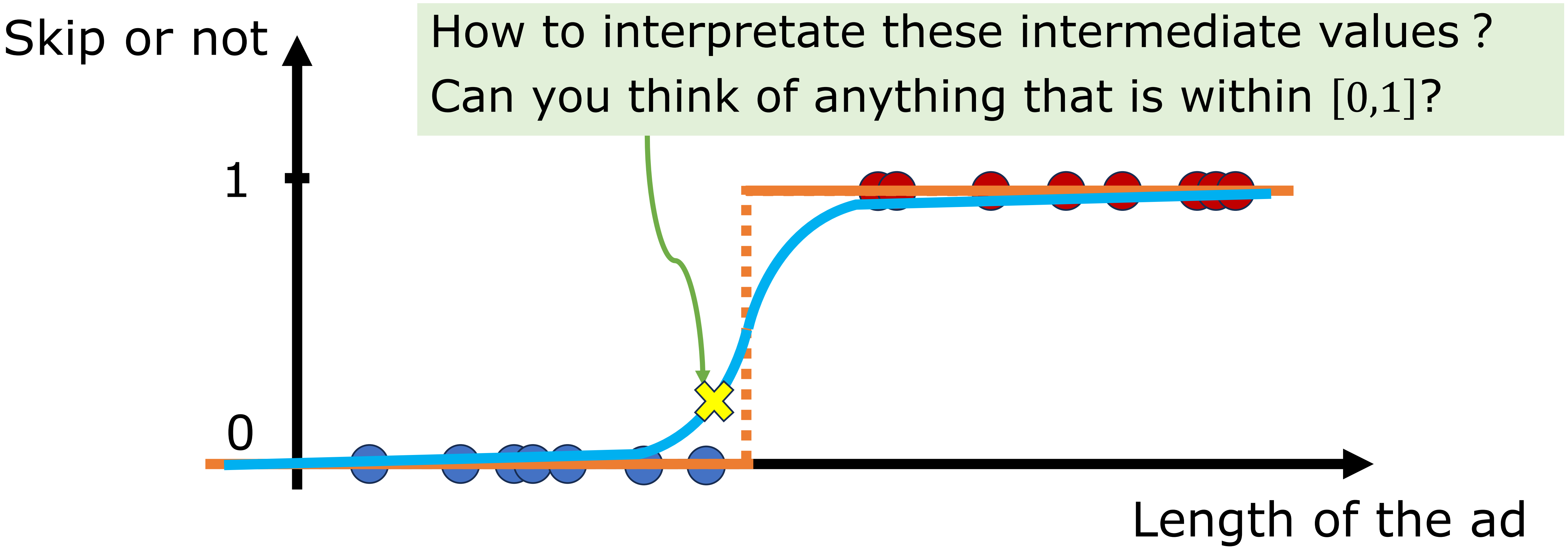
Logistic Functions

- Linear function: $z = wx + b$.
- $H(x) = \sigma(wx + b) = \frac{1}{1+e^{-(wx+b)}}$
- H is the standard logistic function composed with the linear function.

- w: the growth rate
- b: affect the middle point



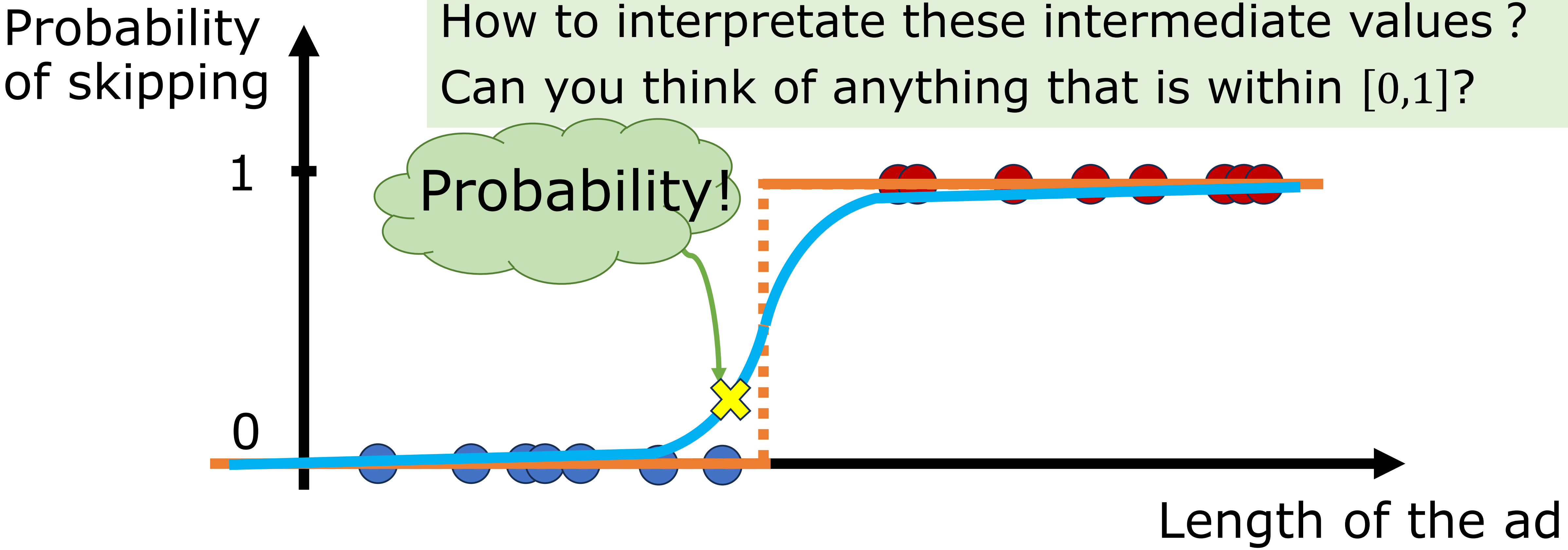
Interpretation: Logistic Functions



Interpretation: Logistic Functions

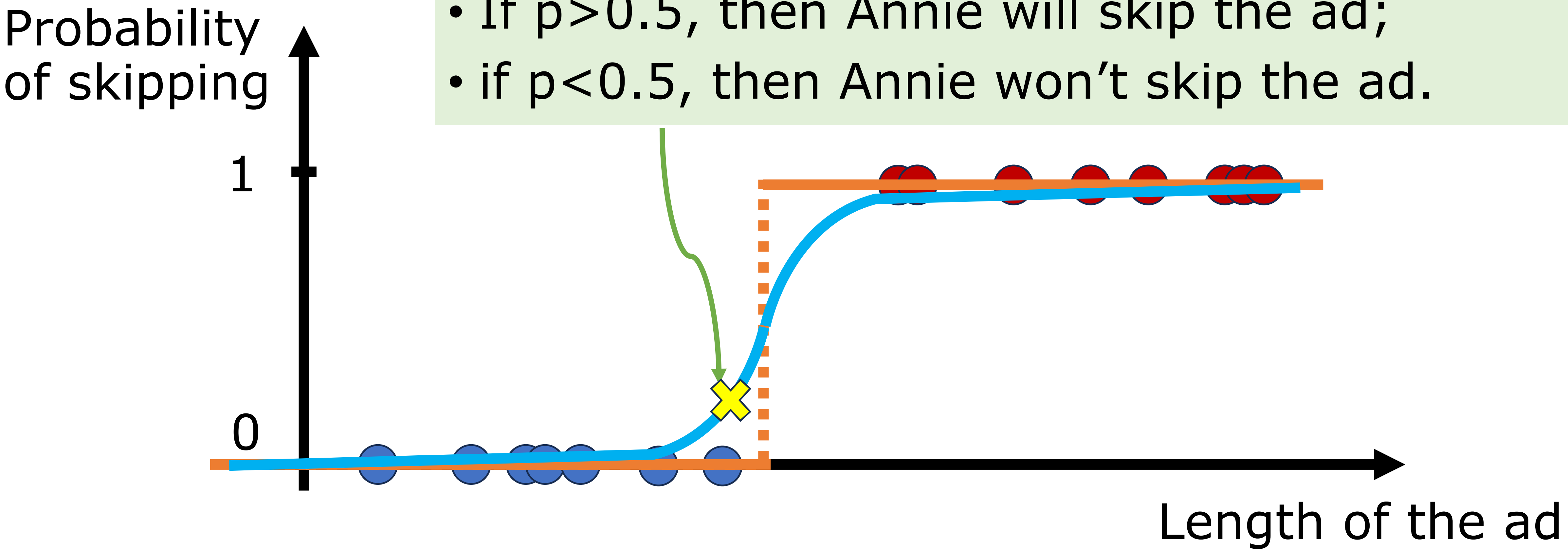
How to interpretate these intermediate values ?

Can you think of anything that is within [0,1]?



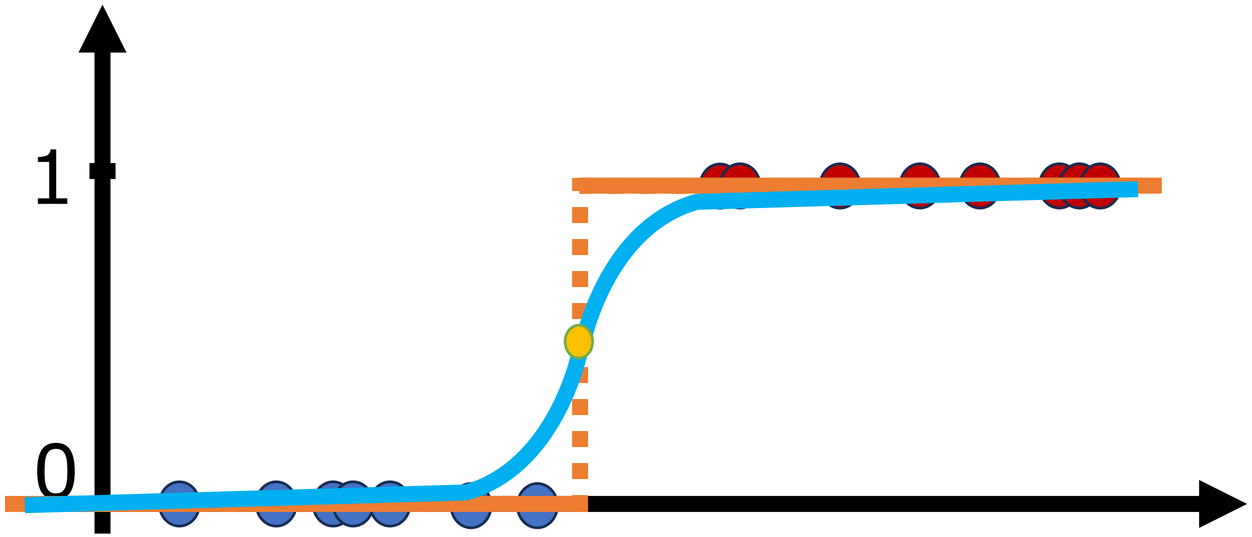
Interpretation: Logistic Functions

- Predict whether Annie will skip the ad.
- Predict the chance that Annie will skip the ad.
- If $p>0.5$, then Annie will skip the ad;
- if $p<0.5$, then Annie won’t skip the ad.



Prediction rules

- $H(x) = \sigma(wx + b) = \frac{1}{1+e^{-(wx+b)}}$
- w: the growth rate; b: affect the middle point
- With different values of w and b, we get different prediction rules.
- Which one is the best?

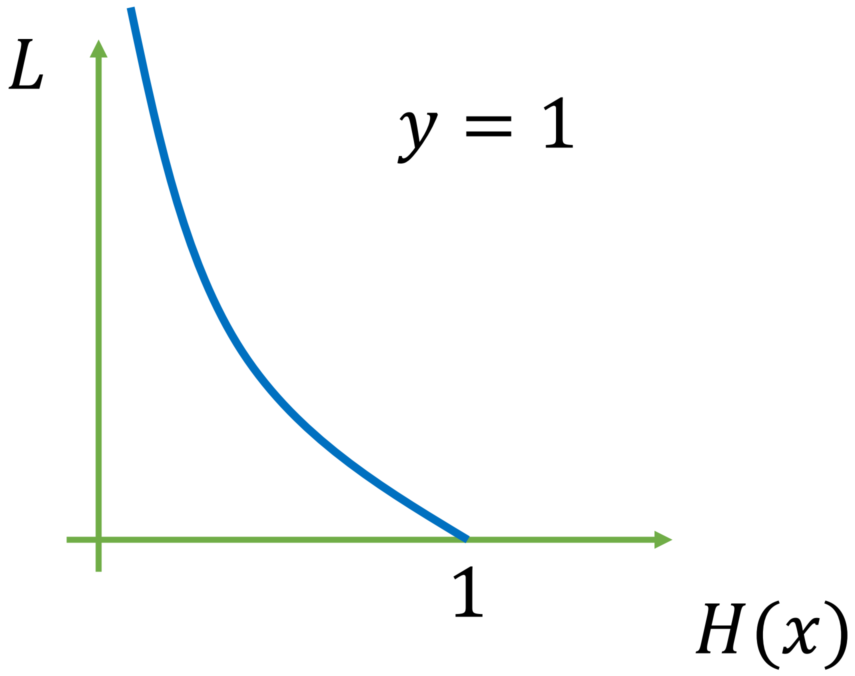


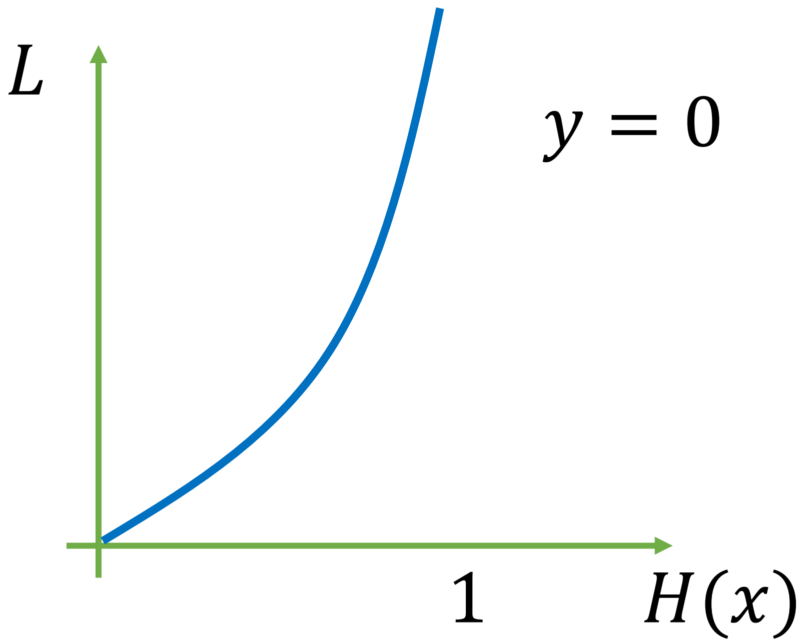
Find the optimal parameters w^*, b^*

- In linear regression, how do we find the best prediction rule?
- We find the prediction line that minimizes the mean square error (MSE)!
- We also need to define a loss function for logistic regression. And the best logistic model is the one that minimizes this loss function.

Loss function

- $L(H(x), y) = \begin{cases} -\ln H(x), & if\ y = 1 \\ -\ln\big(1 - H(x)\big), & if\ y = 0 \end{cases}$





Loss function

- $L(H(x), y) \ = \begin{cases} -\ln H(x), & if\ y = 1 \\ -\ln\big(1 - H(x)\big), & if\ y = 0 \end{cases}$
- These can be combined to a single expression:

$$L(H(x), y) = -y \ln H(x) - (1 - y) \ln\big(1 - H(x)\big)$$

Find the optimal parameters w^*, b^*

- We find w^*, b^* that minimizes the total loss function (log-likelihood).
- Gradient Descent

Regularization and evaluation metrics

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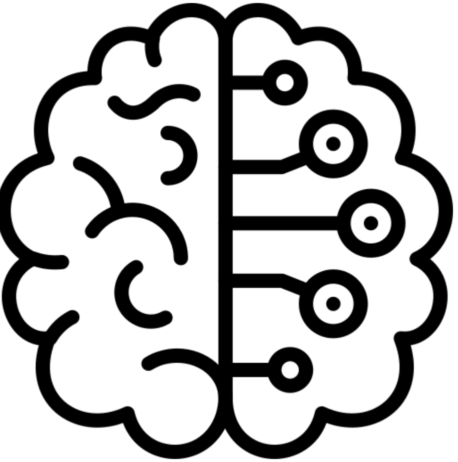
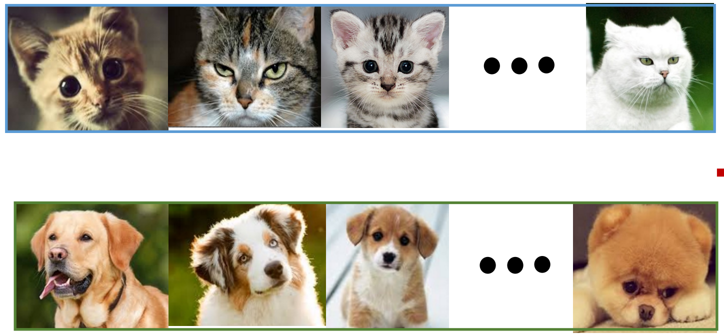
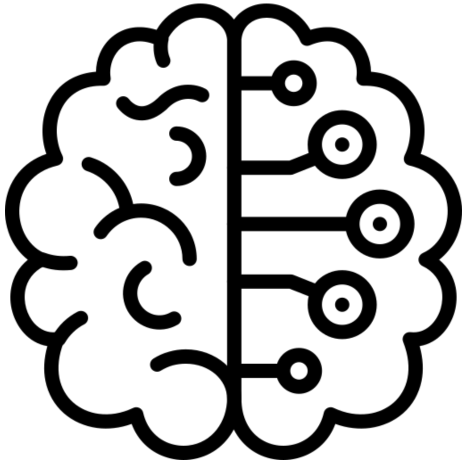
sources used:
1) UCSDX, Prof. Dasgupta fundamentals of machine learning
2) SUT, Prof. Sharifi Zarchi, Introduction to machine learning



Classification problem



Training data

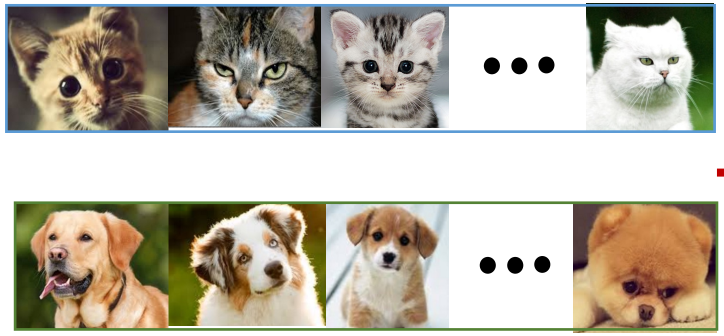


Trained model

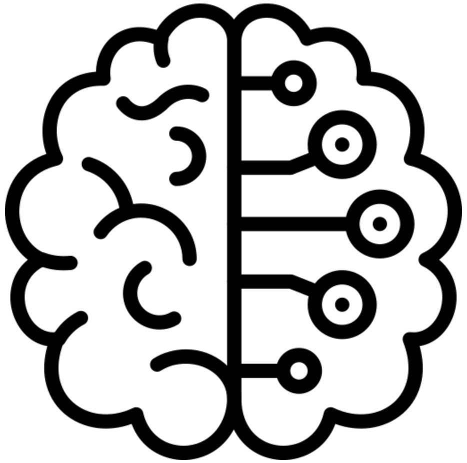
Inference data

Is accuracy the most important evaluation metric?

Accuracy and Confusion Matrix



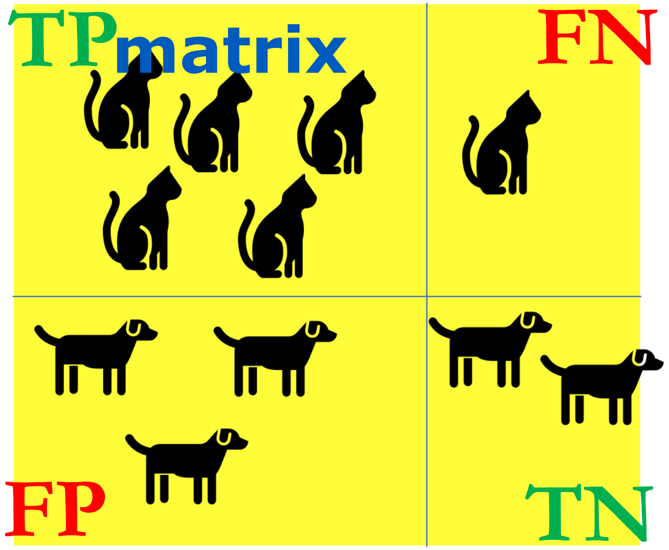
Training data



Trained model

Inference data

Confusion matrix



$$\text{Accuracy} = \frac{TP+TN}{TP+TN+FP+FN}$$

Other metrics

Accuracy is not always the best metric

Let's say we have two tests A and B, their confusion matrix are as following.
Which one is a better test? Whose accuracy is higher?

TP FN

7	3
40	950

FP TN

TP FN

0	10
0	990

FP TN

Other metrics

		Predicted Negative (0)	**Predicted** Positive (1)	
Actual	Negative (0)	**True Negative** **TN**	**False Positive** **FP** (Type I error)	**Specificity** $= \frac{TN}{TN + FP}$
Actual	Positive (1)	**False Negative** **FN** (Type II error)	**True Positive** **TP**	**Recall**, **Sensitivity**, True positive rate (**TPR**) $= \frac{TP}{TP + FN}$
		Accuracy $= \frac{TP + TN}{TP + TN + FP + FN}$	**Precision**, Positive predictive value (**PPV**) $= \frac{TP}{TP + FP}$	**F1-score** $= 2 \times \frac{Recall \times Precision}{Recall + Precision}$

Image source

Precision – recall trade-off

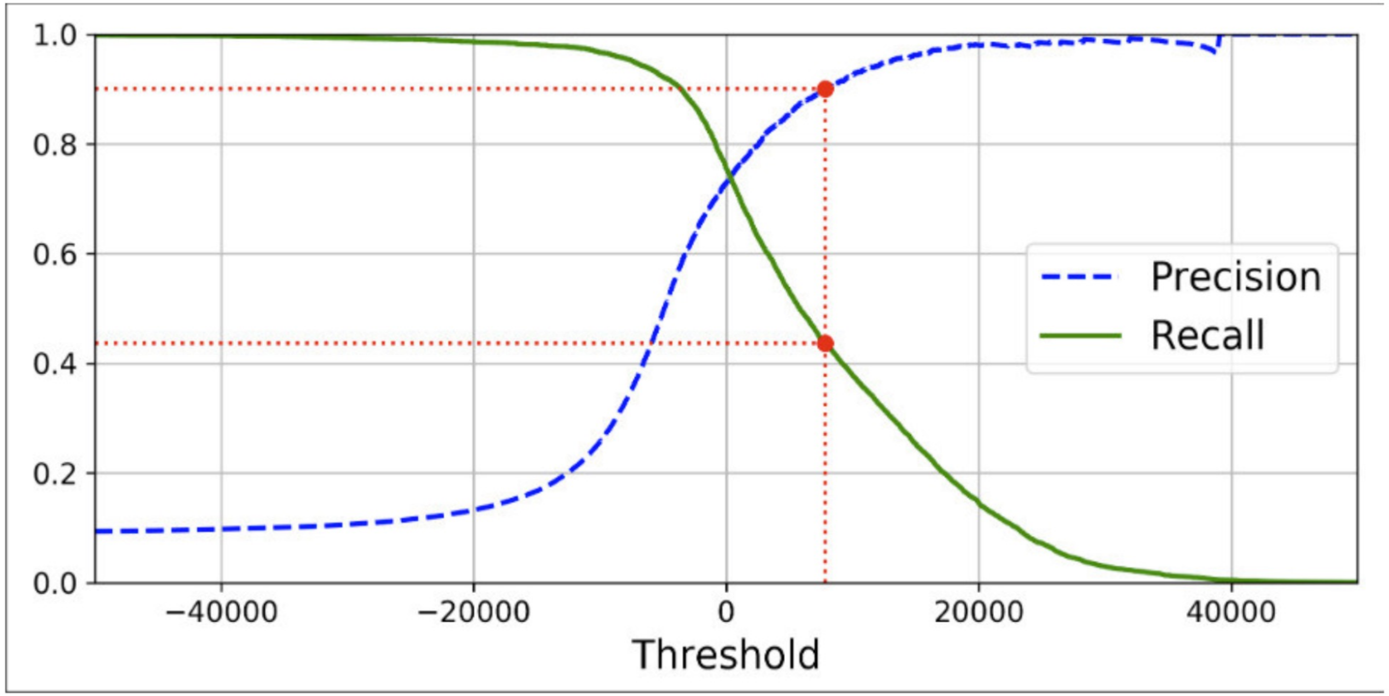


Image source

Other metrics: Area under ROC curve (AUC)

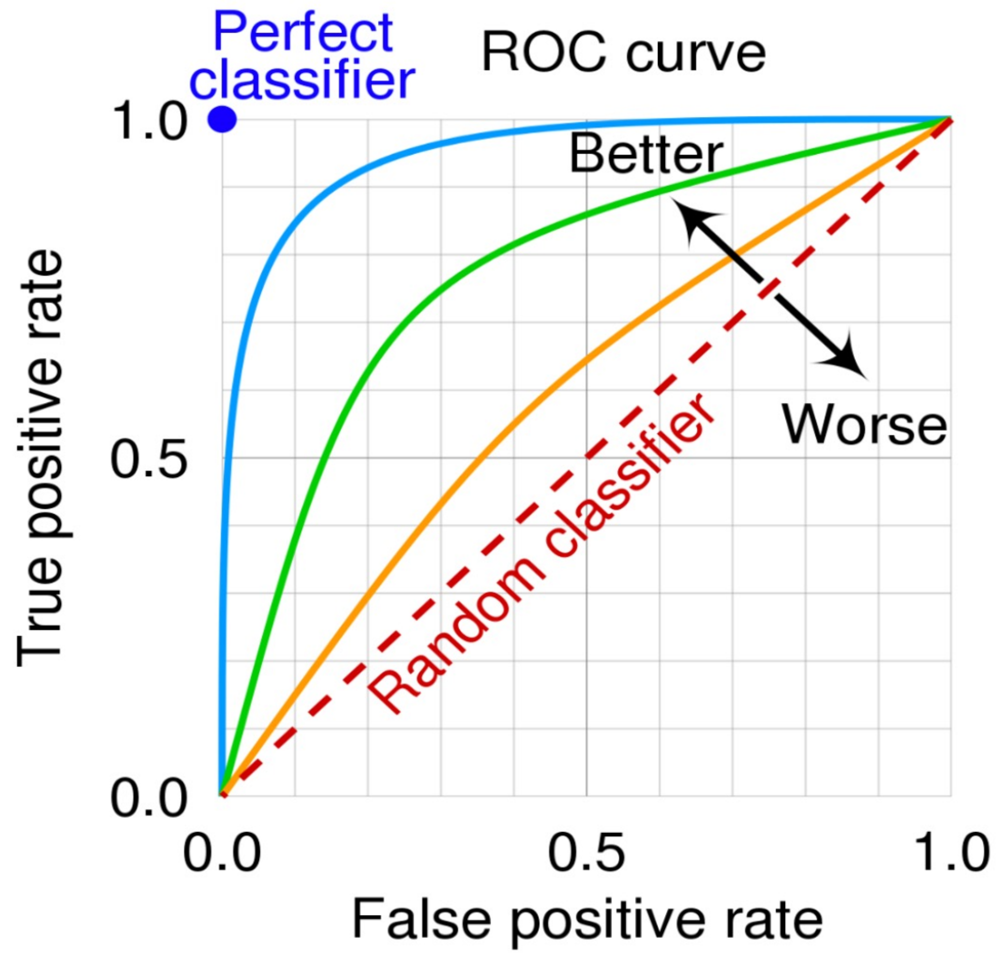
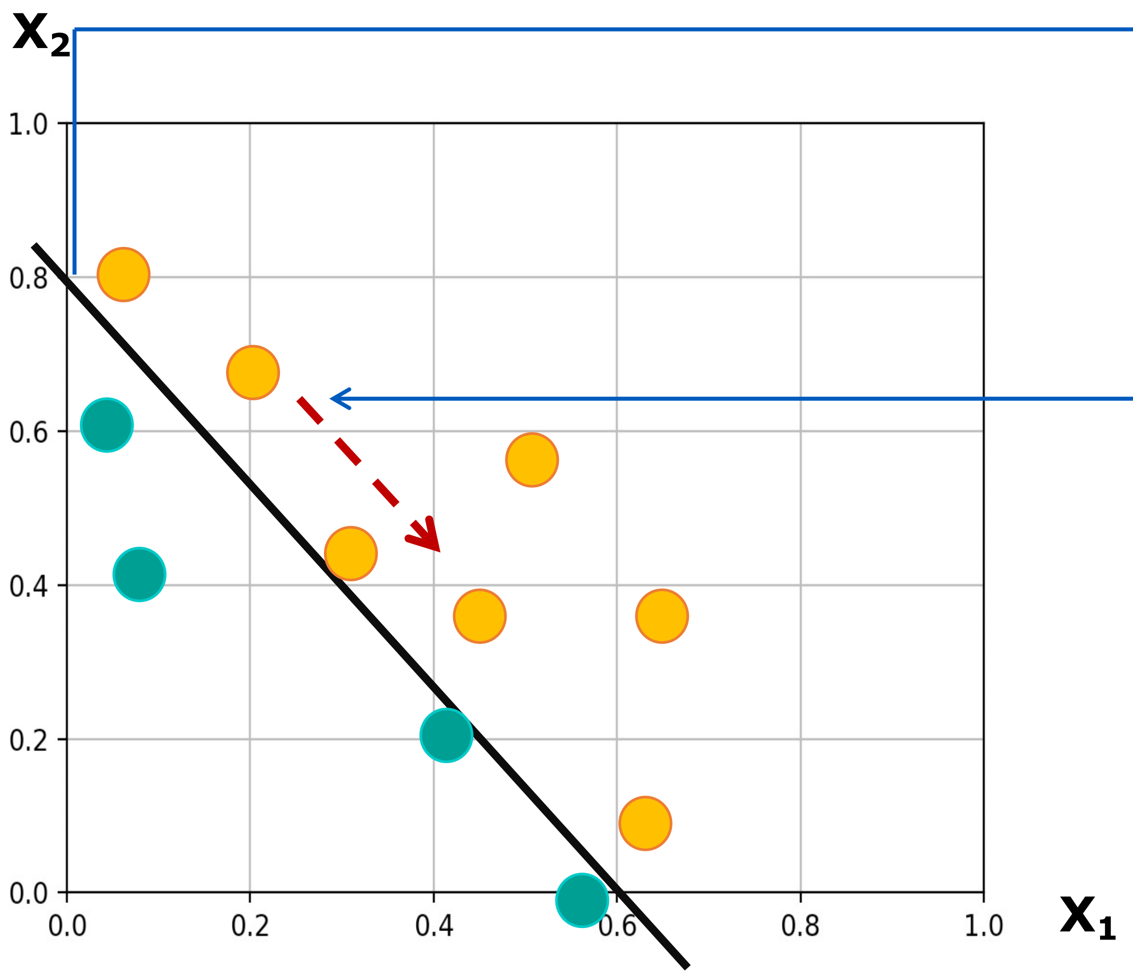


Image source

Simple linear regression



$$y = mx + b$$

b = 0.8

$$m = \frac{0 - 0.8}{0.6 - 0} = \frac{-4}{3}$$

$$y = \frac{-4}{3}\mathrm{x} + \frac{4}{5}$$

Least Square Regression

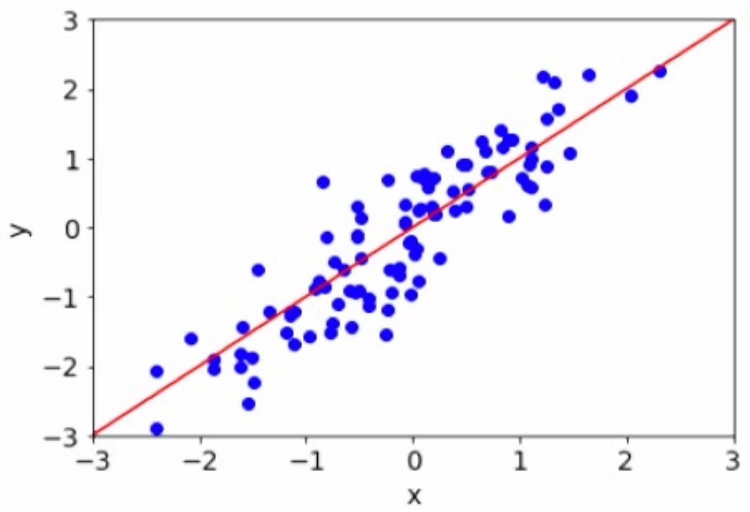
Given a training set $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(n)}, y^{(n)}\right)$, find a linear function, given by $w \in R^d$ and $b \in R$, that minimizes the squared loss:

$$L(w, b) = \sum_{i=1}^{n} (y^i - (w.x^i + b))^2$$

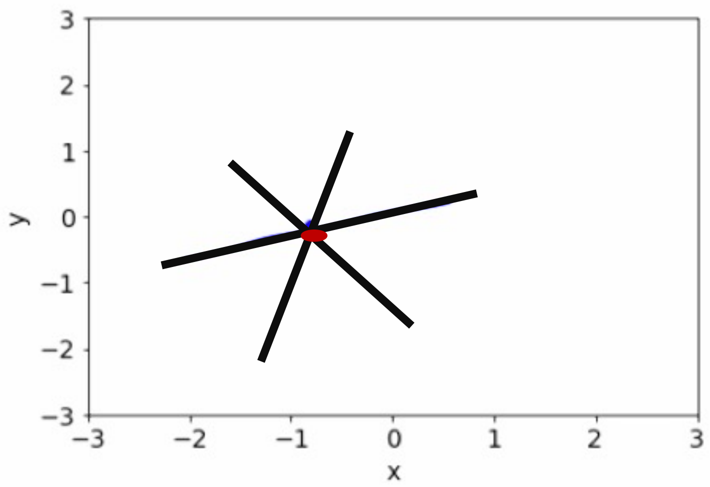
Is training loss a good estimator of future performance?

If n is large enough, maybe
Otherwise, probably an underestimate of future error

Example



n is large given the number of parameters so probably training loss is fine.



We can have multiple different lines and they all will have zero training error, so training loss is not necessarily a good estimator of the performance for future data.

How do we get a good estimate of future error?

k-fold cross validation
Divide the data set into k equal-sized groups $S_1, S_2, \ldots, S_n$
For i=1 to k:
    Train a regressor on all data except S_i
    Let E_i be its error on S_i
Error estimate: average of $E_1, E_2, \ldots, E_k$

But what if training error is not a good measure of future prediction?

Regularization

Minimize squared loss plus a term that penalizes "complex" w:

$$\boldsymbol{L(w,b)} = \sum_{\boldsymbol{i=1}}^{\boldsymbol{n}}(\boldsymbol{y^i} - (\boldsymbol{w.x^i} + \boldsymbol{b}))^2 + \boxed{\lambda||w||^2} \rightarrow \text{regulizer}$$

Adding a penalty term like the above is called regularization

constant $\lambda = 0 \rightarrow$ Least square solution

constant $\lambda \rightarrow\rightarrow \infty \rightarrow$ Only the regulizer matters, we set w=0 (no data)

Example

Given a training set $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(100)}, y^{(100)}\right)$ and the following train/test MSE

λ	training MSE	test MSE	
0.00001	0.00	585.81	$\longrightarrow$ least squares
0.0001	0.00	564.28	
0.001	0.00	404.08	
0.01	0.01	83.48	
0.1	0.03	19.26	
1.0	0.07	7.02	
10.0	0.35	2.84	
100.0	2.40	5.79	
1000.0	8.19	10.97	
10000.0	10.83	12.63	$\longrightarrow$ w is almost 0

Lasso and Ridge Regression

Lasso

$$\boldsymbol{L(w,b)} = \sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} (\boldsymbol{y^i} - (\boldsymbol{w.x^i} + \boldsymbol{b}))^{\boldsymbol{2}} + \boxed{\lambda||w||^2} \rightarrow \text{regulizer}$$

Ridge

$$\boldsymbol{L(w,b)} = \sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} (\boldsymbol{y^i} - (\boldsymbol{w.x^i} + \boldsymbol{b}))^{\boldsymbol{2}} + \boxed{\lambda||w||} \rightarrow \text{regulizer}$$

produces a sparse w
More interpretable and simple

Discussion

1. Why not just use the least squares in logistic regression?
2. What is the difference between “classification” and “regression”?
3. Since logistic regression is an algorithm for classification, why do we call it logistic “regression” instead of logistic “classification”?

1) Least squares is not suitable for logistic regression because it's designed for continuous outcomes, while logistic regression deals with binary probabilities.

2) Classification predicts categorical labels, while regression predicts continuous values.

3) "Logistic regression" is named based on its historical development from linear regression. Logistic regression is a machine learning algorithm that is used to solve Classification problems. Whereas, Linear regression is a machine learning algorithm that is used to solve Regression problems. *Logistic regression is a generalized linear model. And it uses the same basic formula of linear regression* but it is regressing for the probability of a categorical outcome. That’s the reason, logistic regression has “Regression” in its name.

Thank you!