CMPSC 448: Machine Learning

Lecture 10. Logistic Regression

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PennState

Recap: linear models for binary classification

A linear classifier is specified by a weight vector $\boldsymbol{w} \in \mathbb{R}^d$

$$f_{\boldsymbol{w}}(\boldsymbol{x}) = \begin{cases} +1 & \text{if } \ \boldsymbol{w}^\top \boldsymbol{x} = \sum_{i=1}^d w_i x_i \geq 0 \\ -1 & \text{if } \ \boldsymbol{w}^\top \boldsymbol{x} = \sum_{i=1}^d w_i x_i < 0 \end{cases}$$

It will be notationally simpler to use {+1, -1} instead of {1, 0}

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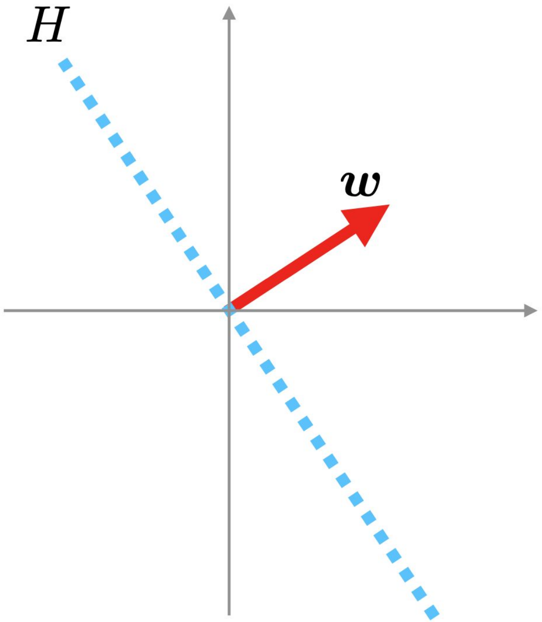
Interpretation: does a linear combination of input features exceed 0?

For $\boldsymbol{w} = [w_1, w_2, \ldots, w_d]^\top$ and $\boldsymbol{x} = [x_1, x_2, \ldots, x_d]^\top$

$$\boldsymbol{w}^\top \boldsymbol{x} = \sum_{i=1}^d w_i x_i >^{?} 0$$

Geometry of linear models for classification



A hyperplane in $\mathbb{R}^d$ is a linear subspace:

A $\mathbb{R}^2$-hyperplane is a line

A $\mathbb{R}^3$-hyperplane is a plane

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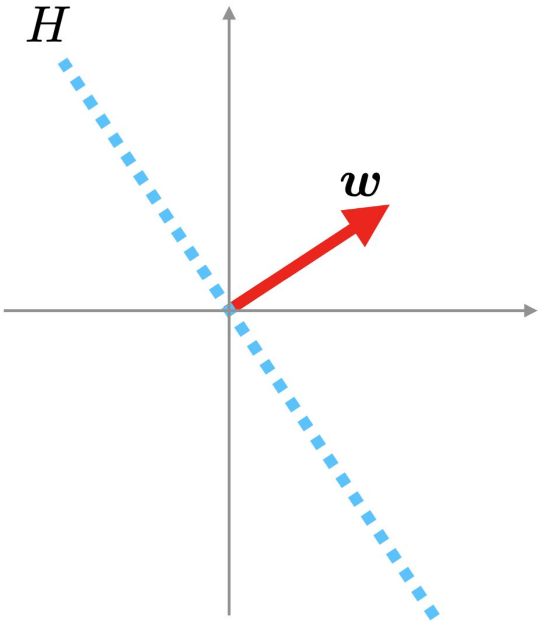

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$$\boldsymbol{w} \in \mathbb{R}^d, \|\boldsymbol{w}\|_2 = 1$$

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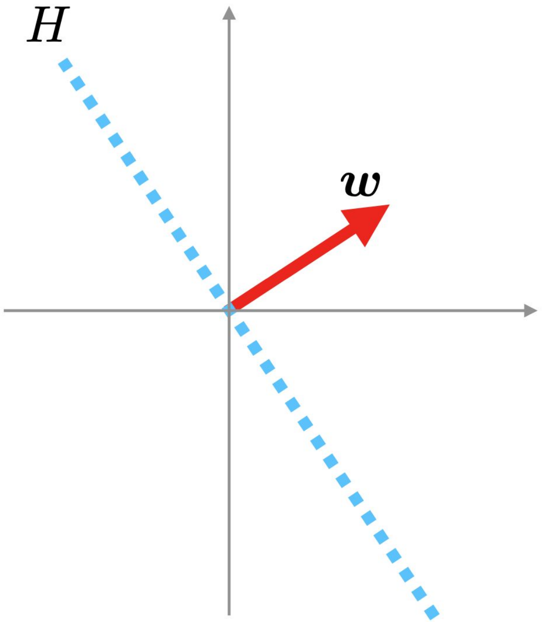

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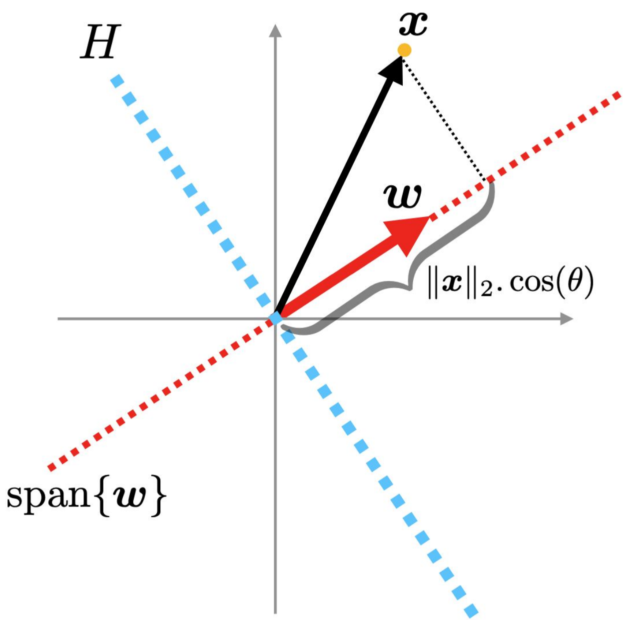
$$\boldsymbol{w} \in \mathbb{R}^d, \ \|\boldsymbol{w}\|_2 = 1$$

The hyperplane with normal vector can be represented by set of points orthogonal to its normal vector:

$$H = \{\boldsymbol{x} \in \mathbb{R}^d \ : \ \boldsymbol{w}^\top \boldsymbol{x} = 0\}$$

Classification using linear models



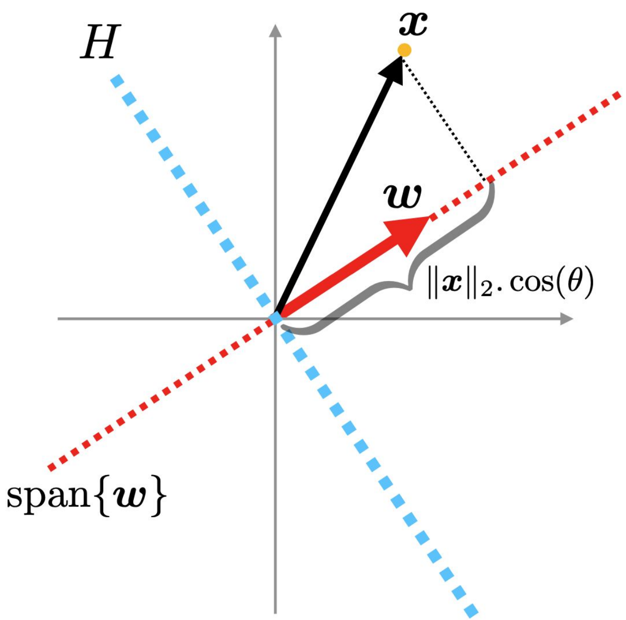
- Projection of $\boldsymbol{x}$ onto $\mathrm{span}\{\boldsymbol{w}\}$ (a line) has coordinate

$$\|\boldsymbol{x}\|_2 \cos(\theta)$$

where

$$\cos(\theta) = \frac{\boldsymbol{w}^\top \boldsymbol{x}}{\|\boldsymbol{w}\|_2 \|\boldsymbol{x}\|_2}$$

Classification using linear models



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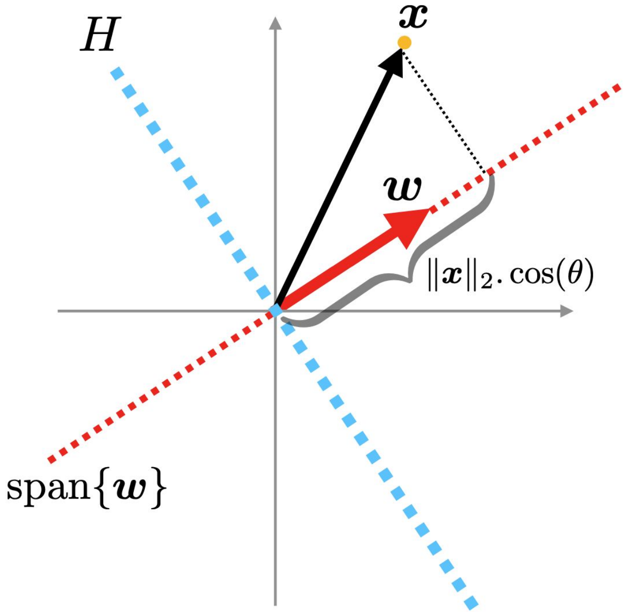
- Decision boundary is hyperplane oriented by $\boldsymbol{w}$

$$\begin{aligned} & \boldsymbol{w}^\top \boldsymbol{x} > 0 \\ \iff & \|\boldsymbol{x}\|_2 \cos(\theta) > 0 \\ \iff & \boldsymbol{x} \text{ on same side of } H \text{ as } \boldsymbol{w} \end{aligned}$$

Classification using linear models



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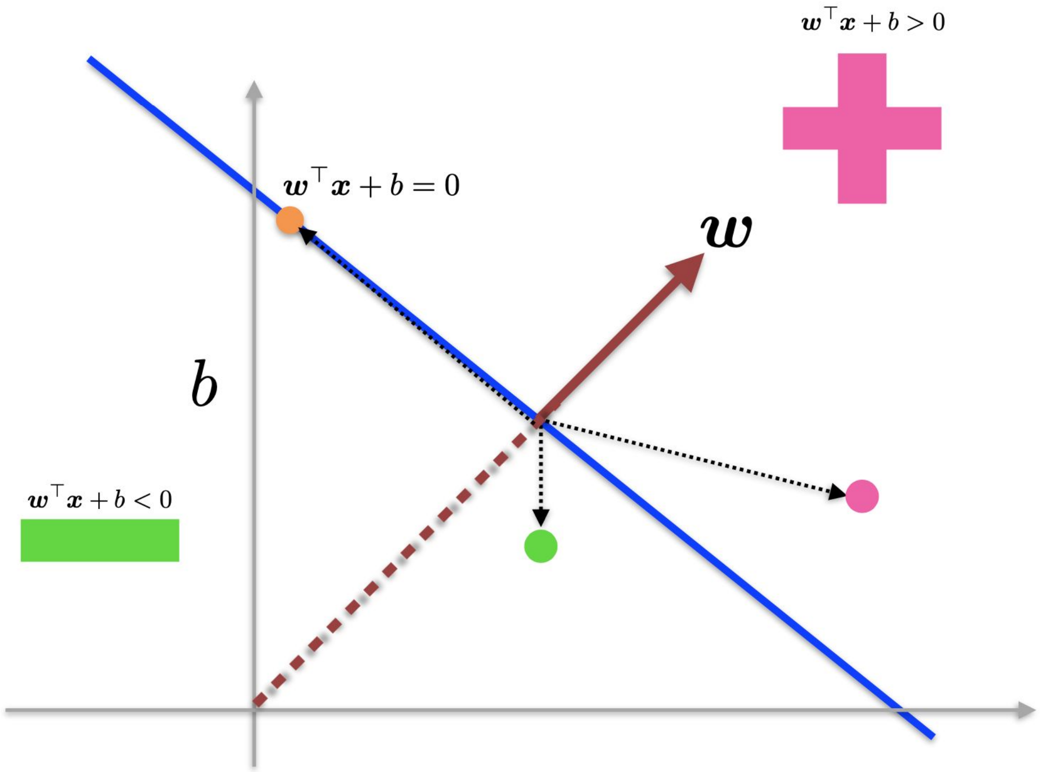
Q: What should we do if we want hyperplane decision boundary that does not (necessarily) go through origin?
A: Add bias.

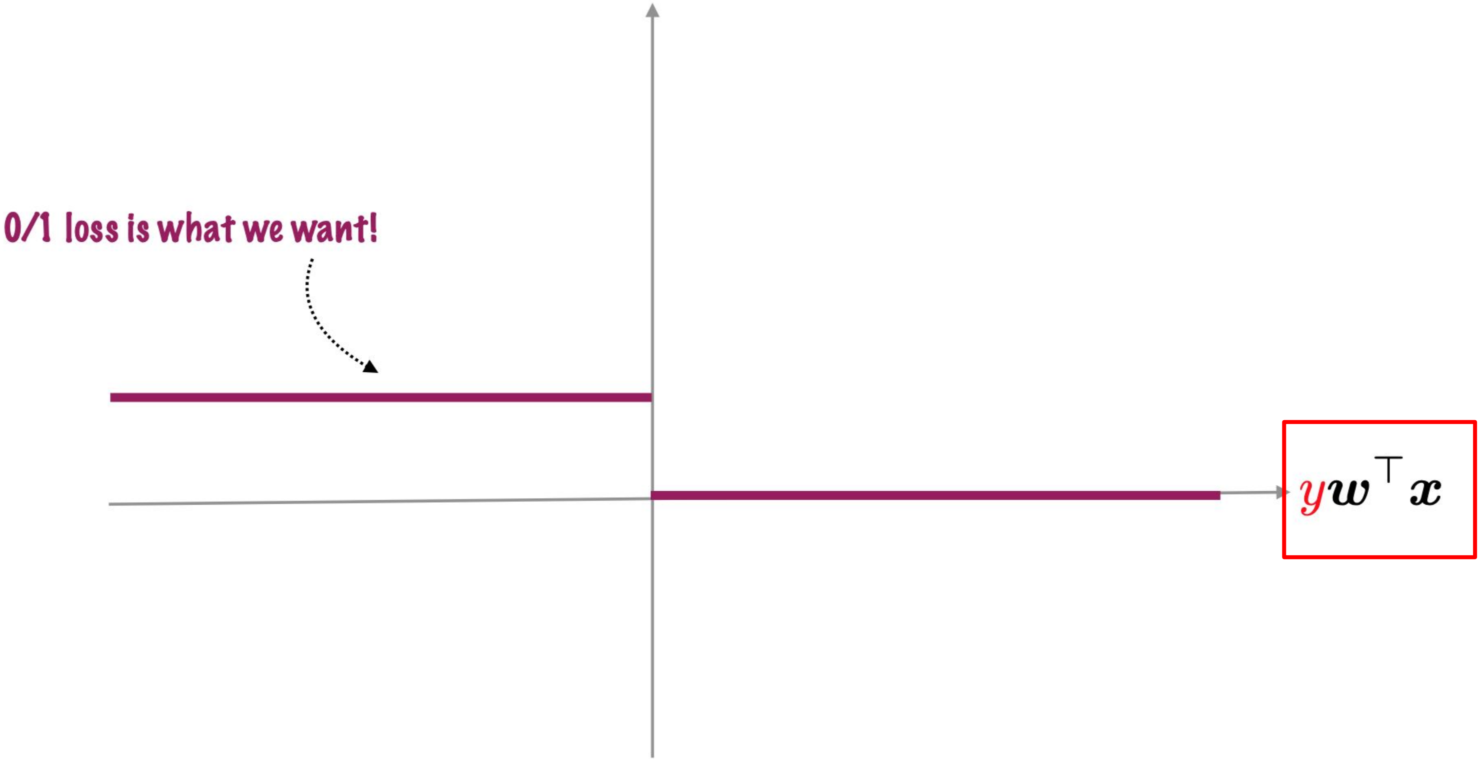
Linear models and hyperplanes

Every hyperplane is a decision boundary that splits the space into two subspaces:



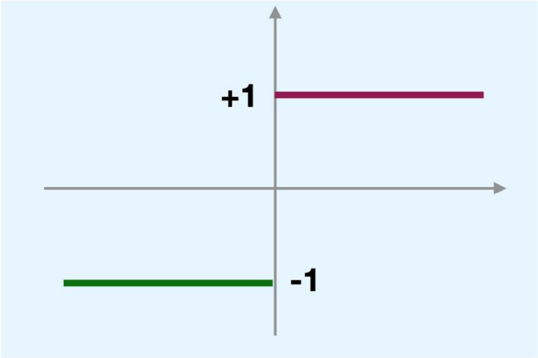
0/1 loss for classification

Combining two cases results in the 0/1 loss function for classification:



Perceptron as an artificial neuron

Perceptron is an **algorithm** to <u>learn</u> **linear models**!

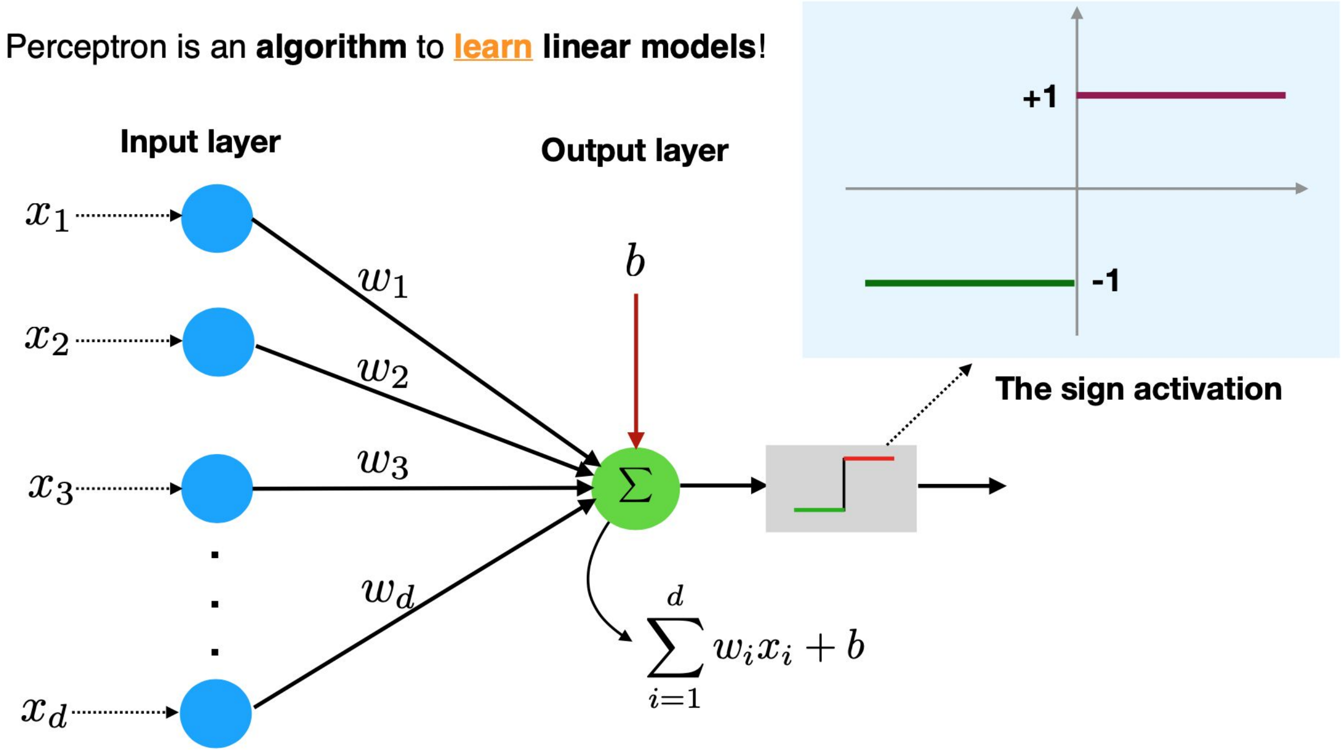


The sign activation

$$\sum_{i=1}^{d} w_i x_i + b$$

It only works if the data is linearly separable (an assumption that does not hold for many real data)

Perceptron as an artificial neuron



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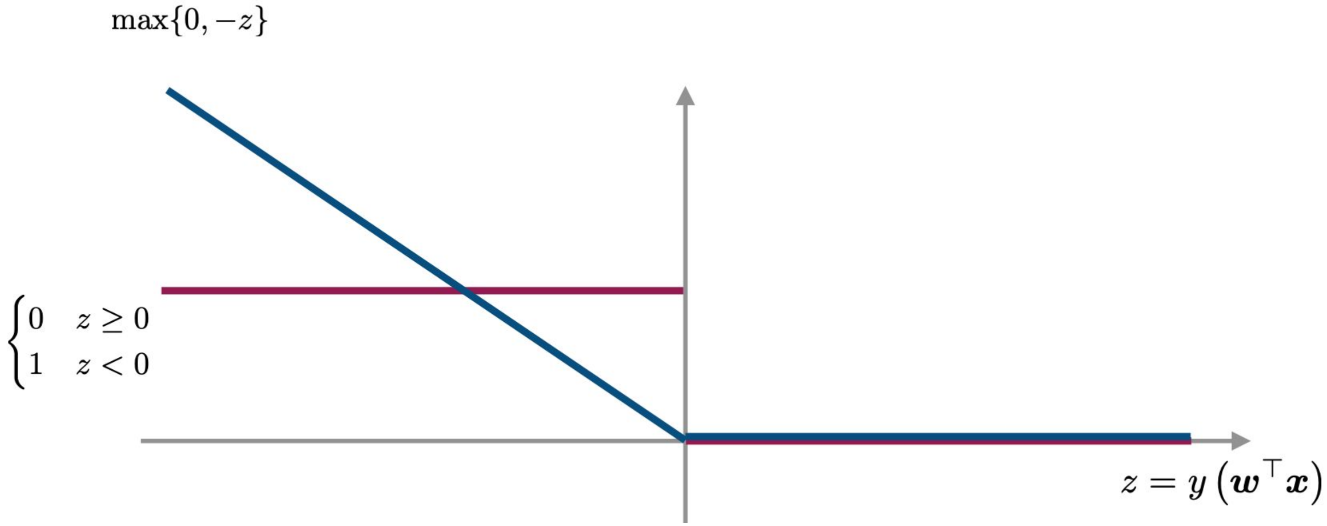
Convex approximation of 0/1 loss

- We want 0/1 loss for classification
- Unfortunately 0/1 loss function is hard to optimize
  - is a non-convex function
  - The gradient is zero
- Let's replace 0/1 loss with approximate convex functions!

The Perceptron loss versus 0/1 loss

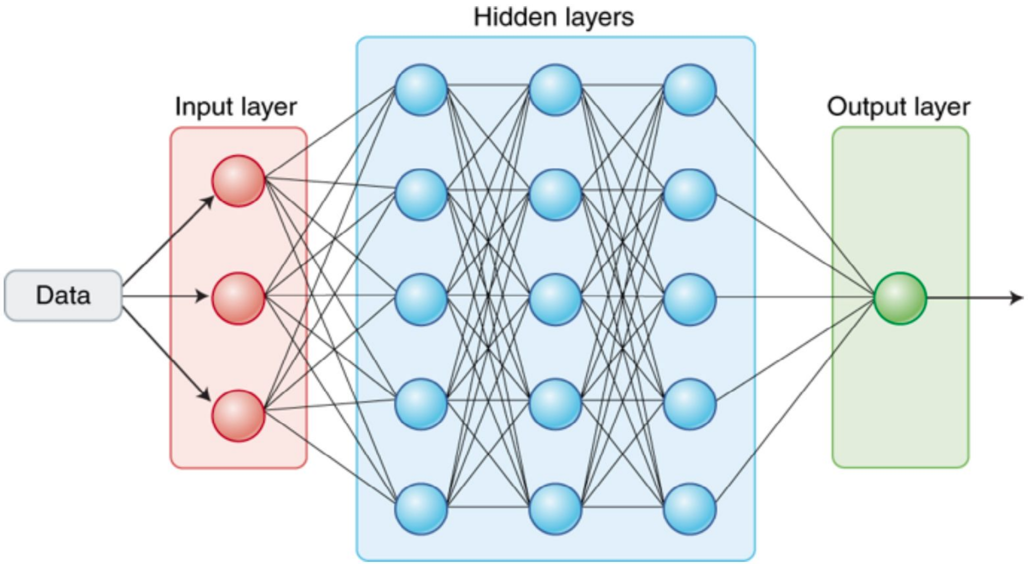
The Perceptron algorithm is optimizing the following loss function in training:

$$\max\{0, -y\left(\boldsymbol{w}^{\top}\boldsymbol{x}\right)\}$$



Computational virtues (convex versus non-convex)

Multiple layer perceptron



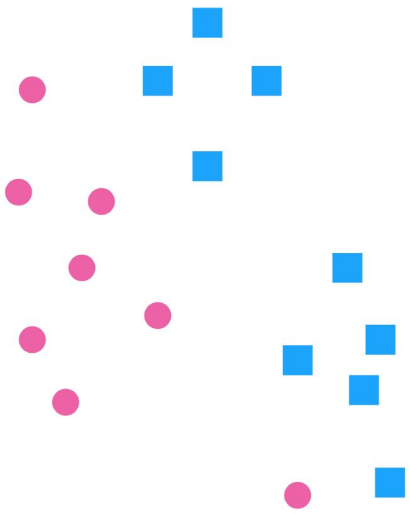
Training: use back-propagation (gradient descent + change rule) to learn the parameters for all layers

Introduces new challenges: huge amount of data + hyperparameter + vanishing gradient issue + high-computational power + more effective regularization + etc

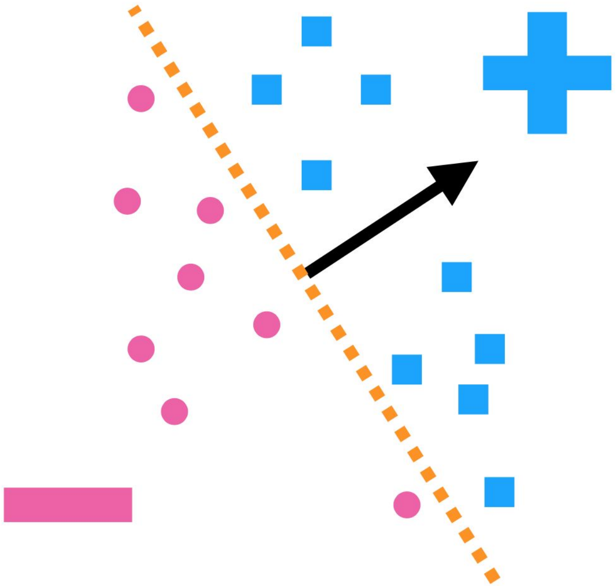
Outline

- Predicting probability
- Logistic regression for binary classification
- MLE for Logistic Regression
- The cross-entropy loss function
- Regularized logistic regression
- The decision boundary of logistic regression

The lack of confidence



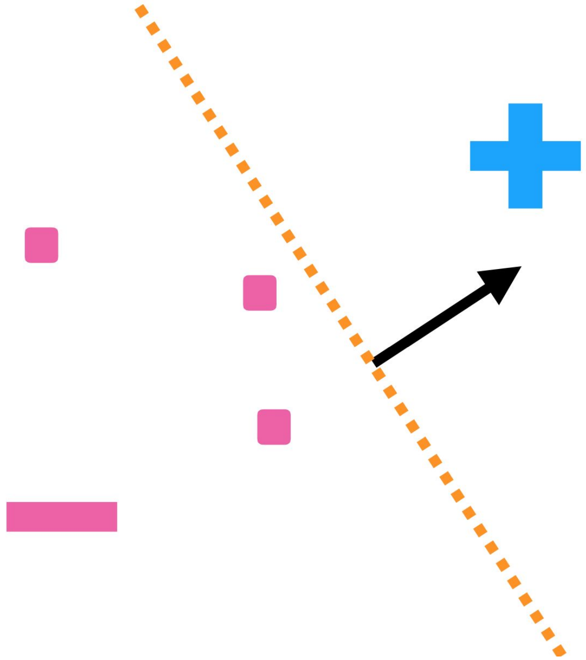
Data



Training

Assume we learn a linear classifier for data given here.

The lack of confidence

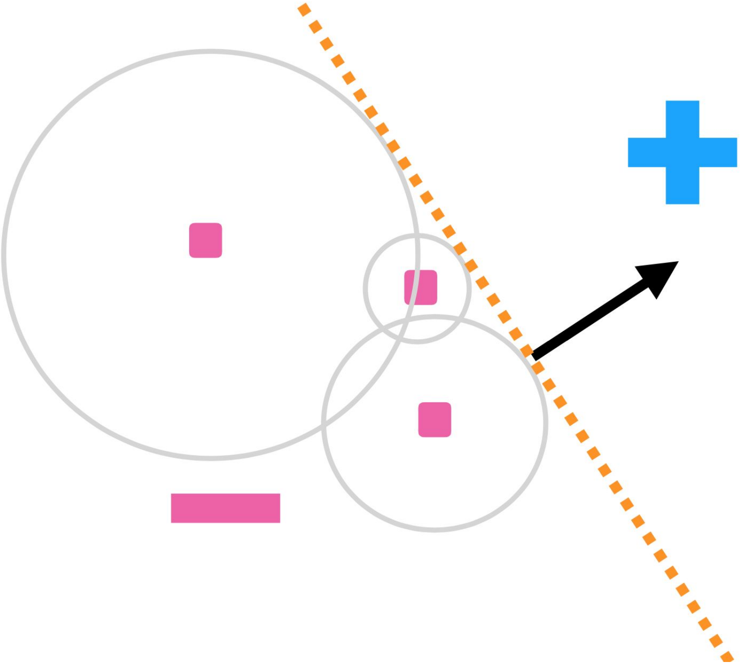


Three test points are given. All will be classifies as -1.

But, which one we are more confident in its label?

Is there any measure of this confidence/probability?

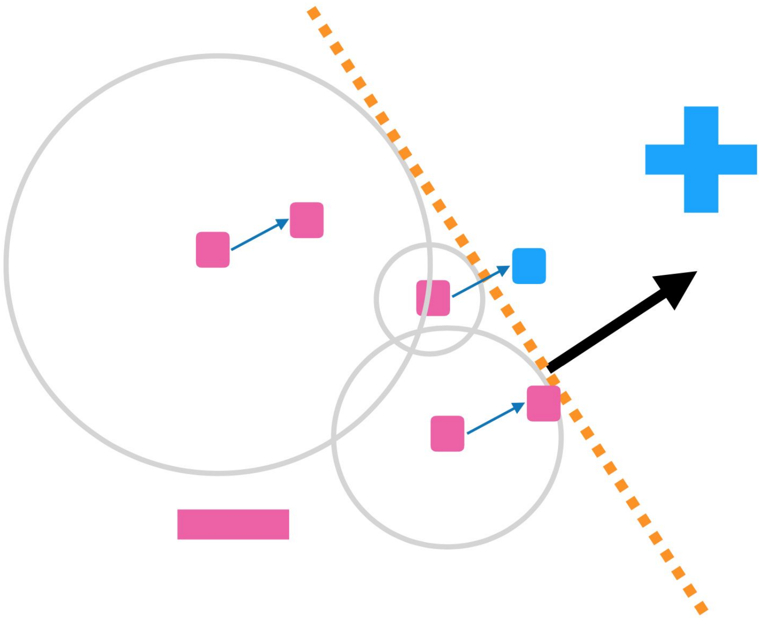
The measure of confidence



The larger the margin (distance from hyperplane), more confidence the algorithm will be in predicted label, which can be computed as

$$y(\boldsymbol{w}^\top \boldsymbol{x})$$

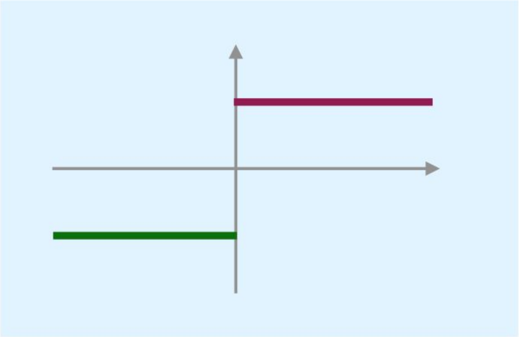
The measure of confidence



Noise tolerance: the amount of noise we can add to each data point such that the label stays same!

From score to probability

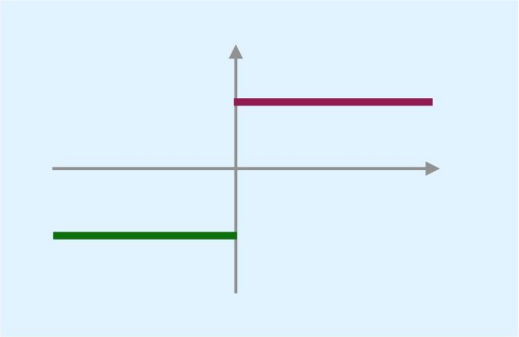
$\boldsymbol{w}^\top \boldsymbol{x}$ →



→ $$y = \begin{cases} +1 & \text{if } \boldsymbol{w}^\top \boldsymbol{x} \geq 0 \\ -1 & \text{if } \boldsymbol{w}^\top \boldsymbol{x} < 0 \end{cases}$$

From score to probability

$$\boldsymbol{w}^\top \boldsymbol{x} \longrightarrow$$



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$$\boldsymbol{w}^\top \boldsymbol{x} \longrightarrow \quad \longrightarrow$$

$$\mathbb{P}[y = +1]$$

$$\mathbb{P}[y = -1] = 1 - \mathbb{P}[y = +1]$$

From score to probability

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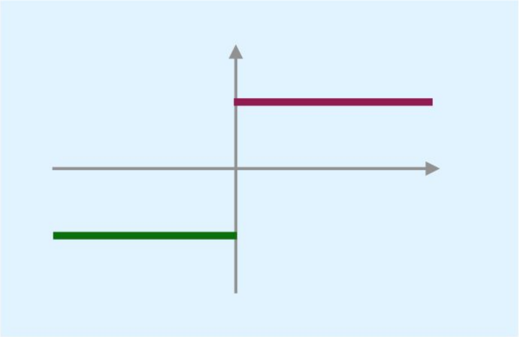

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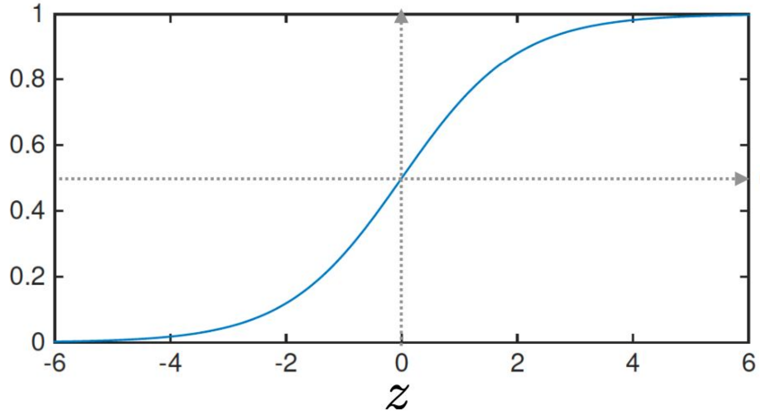
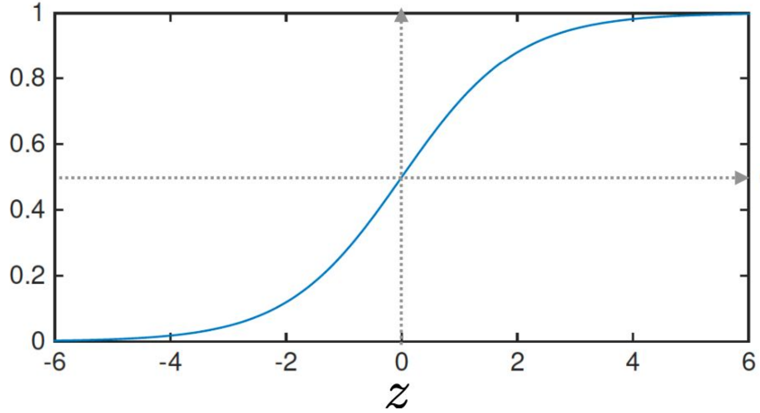


$\mathbb{P}[y = +1 \mid \boldsymbol{x}; \boldsymbol{w}]$

Logistic Function (aka Sigmoid Function)

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

$$\boldsymbol{w}^\top \boldsymbol{x} \longrightarrow$$



$$\longrightarrow \mathbb{P}[y = +1 \mid \boldsymbol{x}; \boldsymbol{w}]$$

$$\begin{aligned} &\mathbb{P}\left[y = +1 | \boldsymbol{x}; \boldsymbol{w}\right] \\ &= \sigma(\boldsymbol{w}^\top \boldsymbol{x}) \\ &= \frac{1}{1 + e^{-\boldsymbol{w}^\top \boldsymbol{x}}} \end{aligned}$$

$$\begin{aligned} &\mathbb{P}\left[y = -1 | \boldsymbol{x}; \boldsymbol{w}\right] \\ &= 1 - \mathbb{P}\left[y = +1 | \boldsymbol{x}; \boldsymbol{w}\right] \\ &= \sigma(-\boldsymbol{w}^\top \boldsymbol{x}) = \frac{1}{1 + e^{\boldsymbol{w}^\top \boldsymbol{x}}} \end{aligned}$$

Logistic Function (aka Sigmoid Function)

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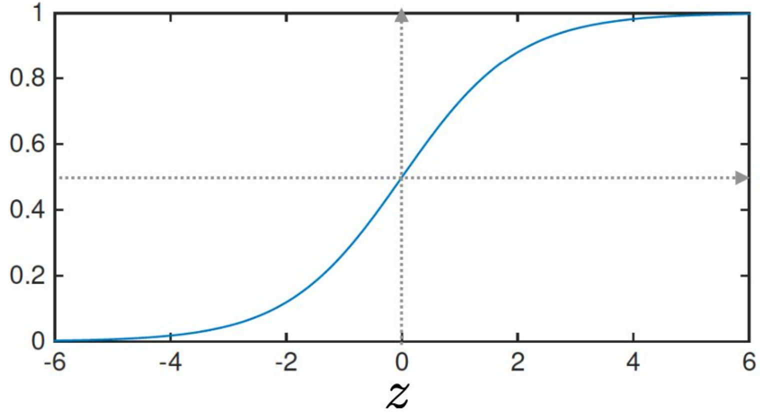
$\boldsymbol{w}^\top \boldsymbol{x} \rightarrow$



$\rightarrow \mathbb{P}[y = +1 \mid \boldsymbol{x}; \boldsymbol{w}]$

$$\boxed{\mathbb{P}\left[y|\boldsymbol{x};\boldsymbol{w}\right] = \frac{1}{1+e^{-y\boldsymbol{w}^\top \boldsymbol{x}}}}$$

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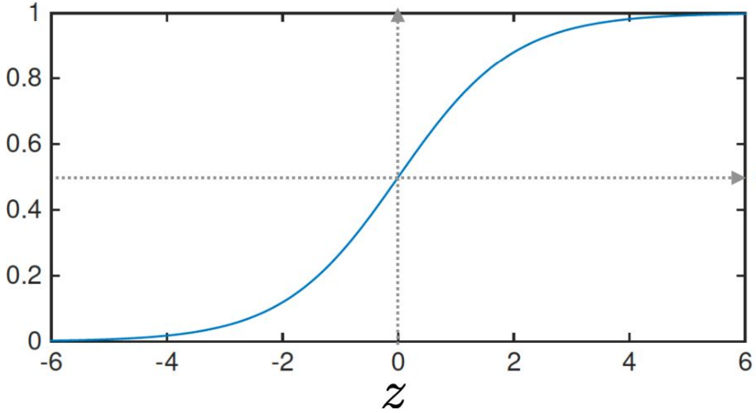

→ $\mathbb{P}[y = +1 \mid \boldsymbol{x}; \boldsymbol{w}]$

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

This “squashing function” known as the **logistic function** (or **sigmoid function**) turns linear prediction score into probability!

Logistic Regression

- Given a data for binary classification: $\mathcal{S} = \{(\boldsymbol{x}_1, y_1 = \pm 1), (\boldsymbol{x}_2, y_2 = \pm 1), \ldots, (\boldsymbol{x}_n, y_n = \pm 1)\}$
- The conditional probability of the label given the input example $\boldsymbol{x}$ for a classifier with parameters vector $\boldsymbol{w}$ is expressed as:

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where the $\boldsymbol{w} = \left[w_1, w_2, \ldots, w_d\right]^\top$ are the adjustable parameters.

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- This is the "logistic function" and model is called "logistic regression".

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In the terminology of statistics, this model is known as logistic "regression", although it should be emphasized that this is a model for classification rather than regression.

MLE for logistic regression

We can fit the logistic models using the maximum likelihood estimation (MLE).

$$\mathbb{P}\left[y|\boldsymbol{x};\boldsymbol{w}\right] = \frac{1}{1+e^{-y\boldsymbol{w}^\top \boldsymbol{x}}}$$

Recall training data are independently generated (i.i.d.), so the likelihood is:

$$\mathbb{P}\left[y_1, y_2, \ldots, y_n \mid \boldsymbol{x}_1, \ldots, \boldsymbol{x}_n; \boldsymbol{w}\right] = \prod_{i=1}^{n} \mathbb{P}\left[y_i|\boldsymbol{x}_i;\boldsymbol{w}\right]$$

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The likelihood measures the probability that the data were generated if $\boldsymbol{w}\in\mathbb{R}^d$ was the model to generate the labels in training data!

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The likelihood measures the probability that the data were generated if $\boldsymbol{w} \in \mathbb{R}^d$ was the model to generate the labels in training data!

By maximizing the likelihood over all parameter vectors $\boldsymbol{w} \in \mathbb{R}^d$ we can find the optimal classifier:

$$\arg\max_{\boldsymbol{w}} \quad \prod_{i=1}^{n} \mathbb{P}\left[y_i|\boldsymbol{x}_i;\boldsymbol{w}\right]$$

Fitting logistic regression models using MLE

$$\log\left(\prod_{i=1}^{n}\mathbb{P}\left[y_i|\boldsymbol{x}_i;\boldsymbol{w}\right]\right) = \sum_{i=1}^{n}\log\mathbb{P}\left[y_i|\boldsymbol{x}_i;\boldsymbol{w}\right]$$

$$= \sum_{i=1}^{n}\log\frac{1}{1+e^{-y_i\boldsymbol{w}^\top\boldsymbol{x}_i}}$$

$$\log\frac{1}{z} = -\log z$$

$$= \sum_{i=1}^{n}-\log\left(1+e^{-y_i\boldsymbol{w}^\top\boldsymbol{x}_i}\right)$$

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$$= -\sum_{i=1}^{n}\log\left(1+e^{-y_i\boldsymbol{w}^\top\boldsymbol{x}_i}\right)$$

The final MLE objective becomes (or minimizing the negative likelihood):

$$\arg\max_{\boldsymbol{w}\in\mathbb{R}^d}\ -\sum_{i=1}^{n}\log\left(1+e^{-y_i\boldsymbol{w}^\top\boldsymbol{x}_i}\right) \qquad \arg\min_{\boldsymbol{w}\in\mathbb{R}^d}\ \sum_{i=1}^{n}\log\left(1+e^{-y_i\boldsymbol{w}^\top\boldsymbol{x}_i}\right)$$

The cross-entropy loss function

The cross-entropy function to measure the error of model on a training sample:

$$\log\left(1+e^{-y\boldsymbol{w}^\top\boldsymbol{x}}\right)$$

The cross-entropy loss function

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It looks complicated and ugly, but,

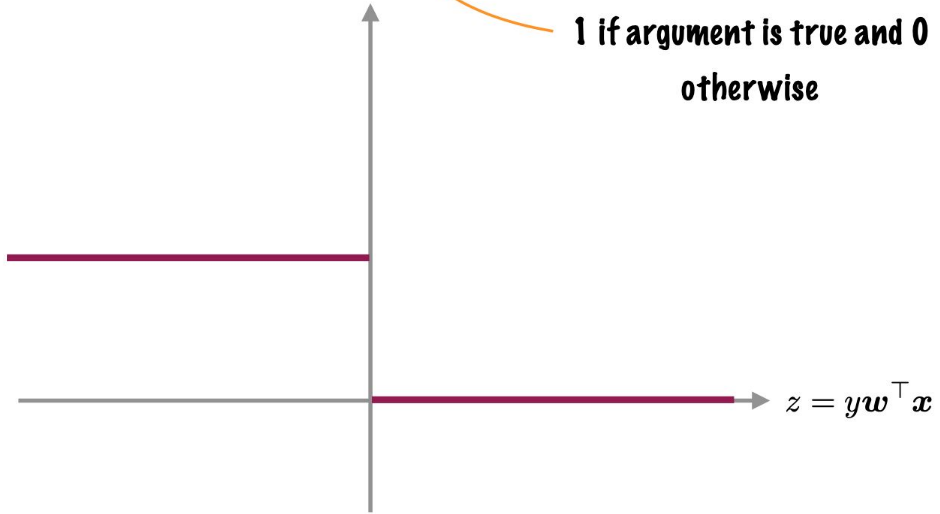
- It is based on an intuitive probabilistic interpretation.
- It is convex.
- However, unlike linear regression, there is no closed-form solution (even though it is convex).
- It is very convenient and mathematically easy to minimize using Gradient Descent (GD).

Optimization viewpoint of linear classifiers

The original goal of linear binary classification is to find the parameters of a linear model that minimizes the number of mistakes over training data (0/1 loss):

$$\arg \min_{\boldsymbol{w} \in \mathbb{R}^d,\ b \in \mathbb{R}} \sum_{i=1}^{n} \mathbb{I}\left[\text{sign}(\boldsymbol{w}^\top \boldsymbol{x} + b) \neq y_i\right]$$

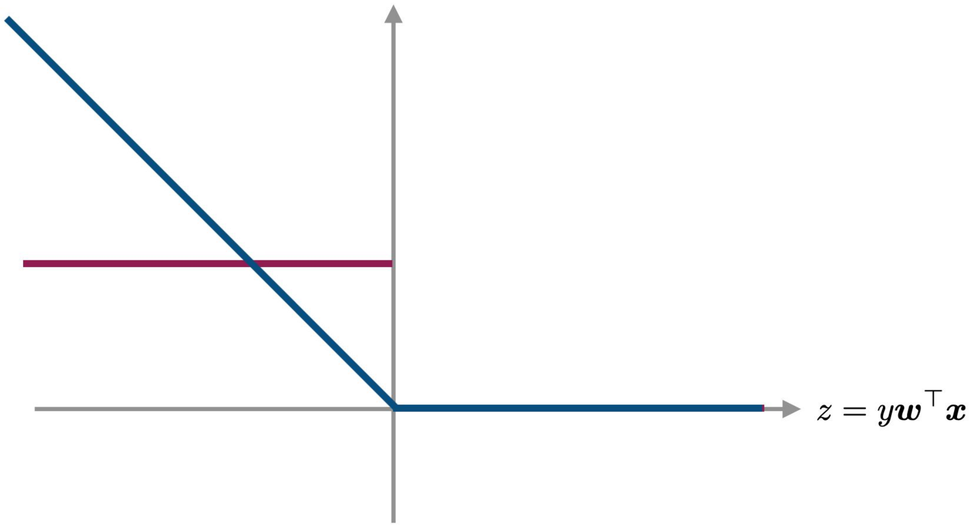
Indicator functions: returns 1 if argument is true and 0 otherwise



Optimization viewpoint of linear classifiers

Perceptron minimizes a convex relaxation version of 0/1 loss:

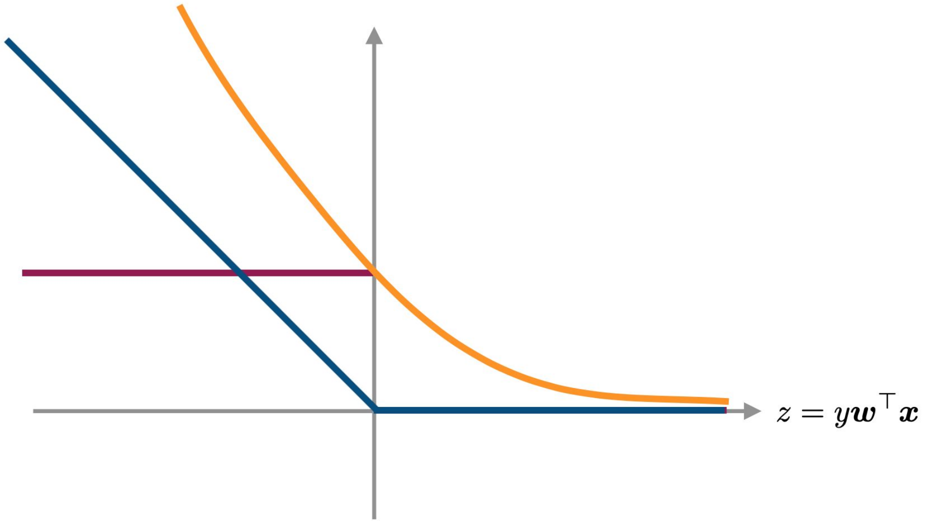
$$\arg\min_{\boldsymbol{w}\in\mathbb{R}^d,\ b\in\mathbb{R}} \sum_{i=1}^{n} \max\left(0, -y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b)\right)$$



Optimization viewpoint of linear classifiers

Logistic regression minimizes another convex relaxation version of 0/1 loss, and it is a smooth version of loss used in Perceptron:

$$\arg\min_{\boldsymbol{w}\in\mathbb{R}^d,\ b\in\mathbb{R}} \sum_{i=1}^{n} \log\left(1+e^{-y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b)}\right)$$

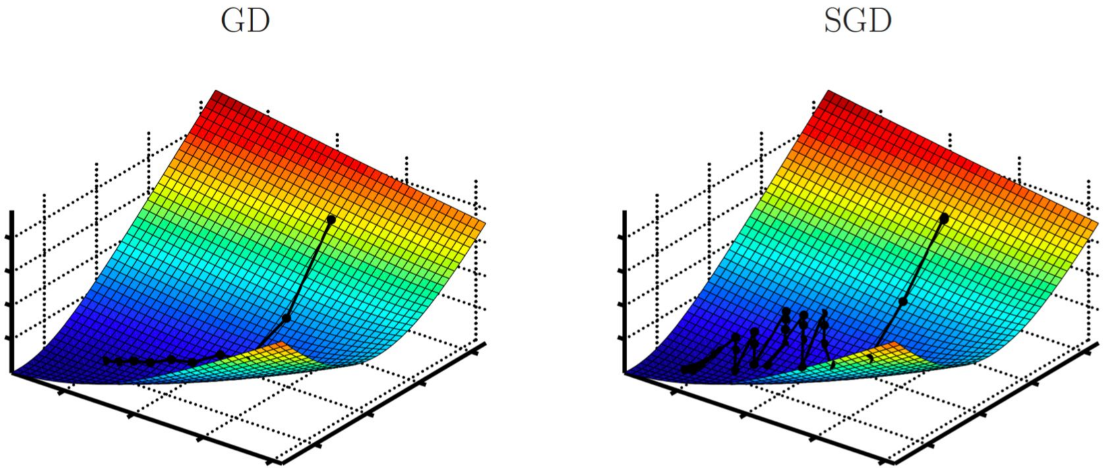


GD and SGD

Our task now is to solve the following optimization problem to find optimal model:

$$\arg\min_{\boldsymbol{w}\in\mathbb{R}^d} \quad \sum_{i=1}^{n} \log\left(1 + e^{-y_i \boldsymbol{w}^\top \boldsymbol{x}_i}\right)$$

The function is a convex function of the parameters and we can use GD or SGD to find the minimizer.



Overfitting in Logistic Regression

MLE can exhibit severe **overfitting** for data sets that are **linearly separable**.

- In fact, there are infinite number separating hyperplanes
- MLE will give solution for weights go to infinity!

$$|\boldsymbol{w}| \to \infty, \quad \text{then we have} \quad P(y_i|\boldsymbol{w}, \boldsymbol{x}_i) = \sigma(y_i \boldsymbol{w}^\top \boldsymbol{x}_i) \to 1$$

Regularization

MLE can exhibit severe **overfitting** for data sets that are **linearly separable**.

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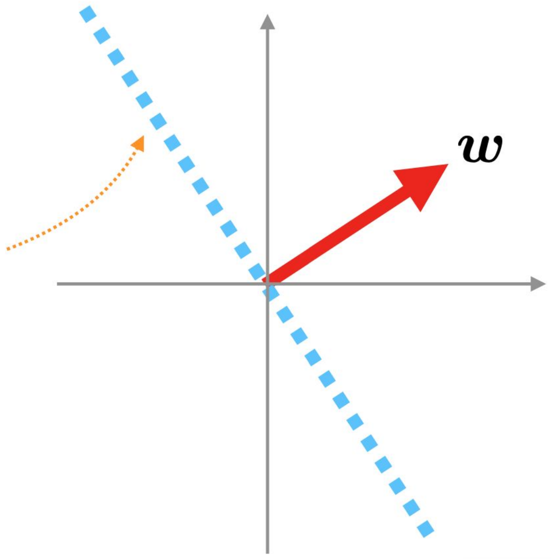
Penalize the model parameters to avoid overfitting:

$$\arg\min_{\boldsymbol{w} \in \mathbb{R}^d} \quad \sum_{i=1}^{n} \log\left(1 + e^{-y_i \boldsymbol{w}^\top \boldsymbol{x}_i}\right) + \lambda \|\boldsymbol{w}\|_2^2$$

The decision boundary

Recall that for Perceptron the decision boundary of a model parametrized by $\boldsymbol{w}$ is the set of all points for which:

$$\boldsymbol{w}^\top \boldsymbol{x} = 0$$



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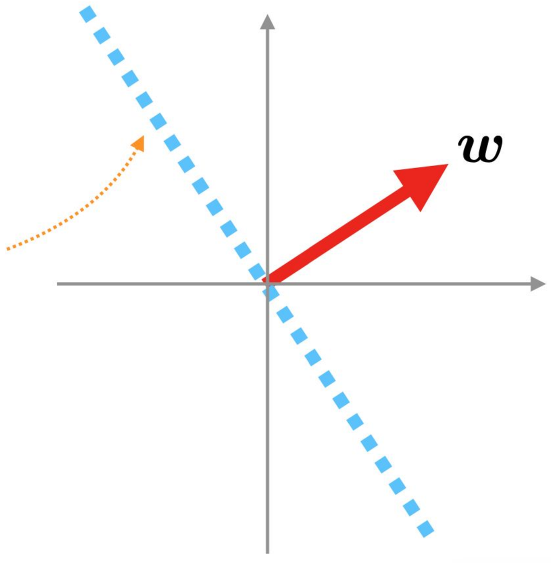


For logistic regression, the decision boundary is the set of all points for which

$$\mathbb{P}[y = -1] = \mathbb{P}[y = +1] = \frac{1}{2}$$

How does the decision boundary for logistic regression look like?

The decision boundary

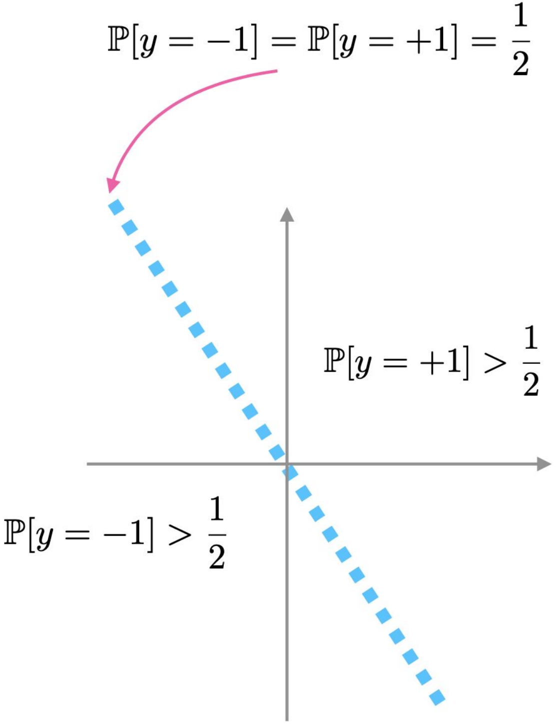
How does the decision boundary for logistic regression look like?

$$\mathbb{P}[y=+1] = \frac{1}{1+e^{-\boldsymbol{w}^\top \boldsymbol{x}}} = \frac{1}{2}$$

$$e^{-\boldsymbol{w}^\top \boldsymbol{x}} = 1$$

$$-\boldsymbol{w}^\top \boldsymbol{x} = 0$$

$$\boldsymbol{w}^\top \boldsymbol{x} = 0$$



The decision boundary of logistic regression is linear!

Note on Label Notations

In this class note, we use

$$\mathcal{Y} = \{-1, +1\}$$

It is also possible (and actually, more popular) to use

$$\mathcal{Y} = \{0, 1\}$$

You will work with this setting in your HW3.

Perceptron versus logistic regression

	Perceptron	Logistic regression
Model	$\boldsymbol{w}^\top \boldsymbol{x} + b$	$\boldsymbol{w}^\top \boldsymbol{x} + b$
Prediction	$\mathrm{sign}(\boldsymbol{w}^\top \boldsymbol{x} + b)$	$\sigma(\boldsymbol{w}^\top \boldsymbol{x} + b)$
Training loss function	$\max\left(0, -y(\boldsymbol{w}^\top \boldsymbol{x} + b)\right)$	$\log\left(1 + e^{-y(\boldsymbol{w}^\top \boldsymbol{x} + b)}\right)$
Decision boundary	Linear	Linear
Regularization	NA (data needs to be separable)	$\|\boldsymbol{w}\|_2^2$ or $\|\boldsymbol{w}\|_1$
Optimization	GD + SGD	GD + SGD

Logistic regression in scikit-learn

```
from sklearn.linear_model import LogisticRegression
from sklearn.cross_validation import train_test_split

# Assume data are in X (features) and y (binary labels)
# Scikit Logistic Regression
scikit_log_reg = LogisticRegression()
scikit_log_reg.fit(X, y)
```