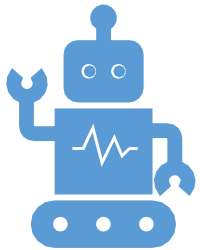




UiO : **University of Oslo**

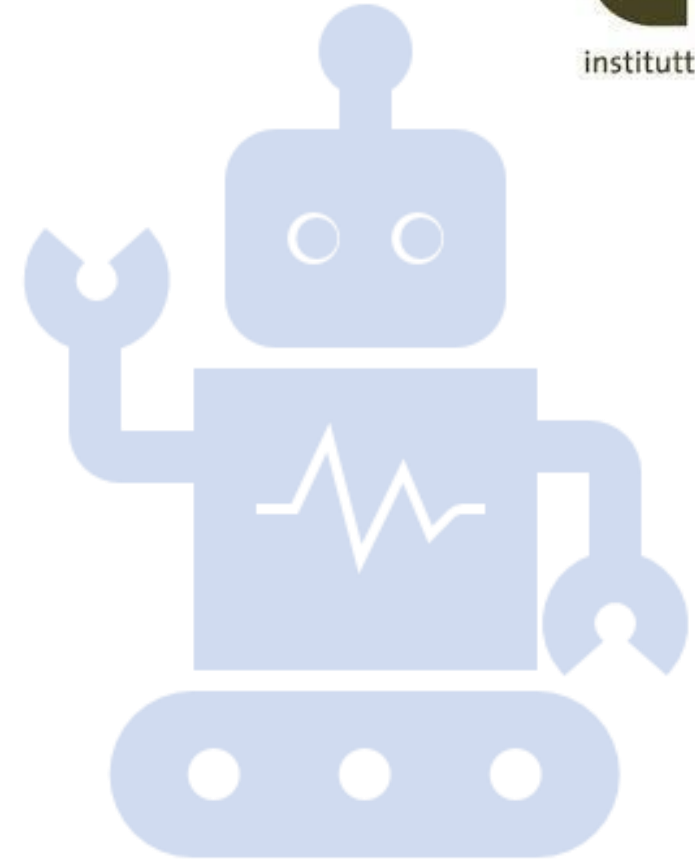


IN3050/IN4050 - Introduction to Artificial Intelligence and Machine Learning

Lecture 7 – 2021

Logistic Regression

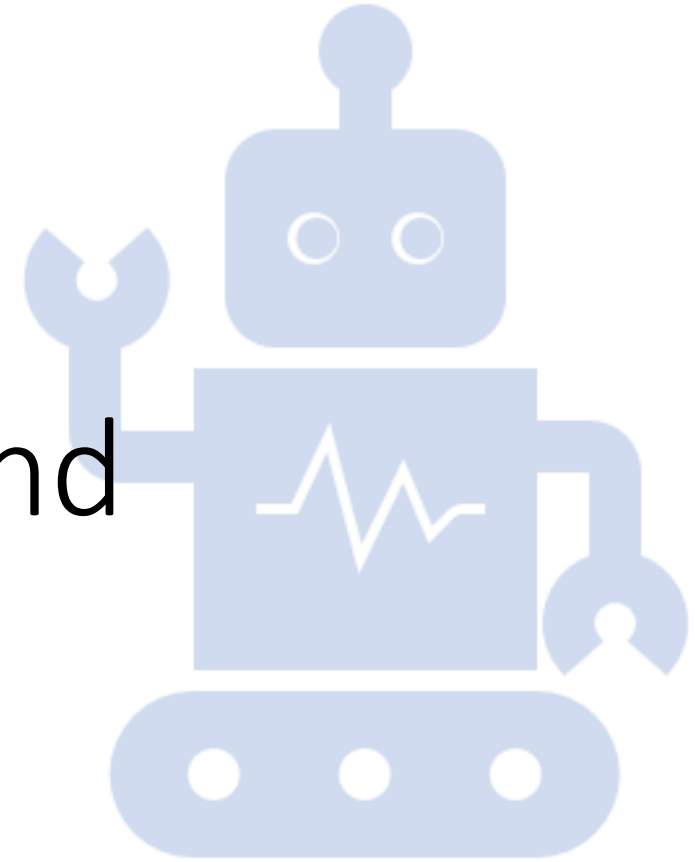
Jan Tore Lønning





7.1 Linear Regression and Classification

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Today

1. Linear Regression and Classification
2. The Logistic Function and its Derivative
3. The Logistic Regression Classifier
4. Cross-Entropy Loss
5. Training the Logistic Regression Classifier
6. Variants of Gradient Descent
7. Multi-Class Classification

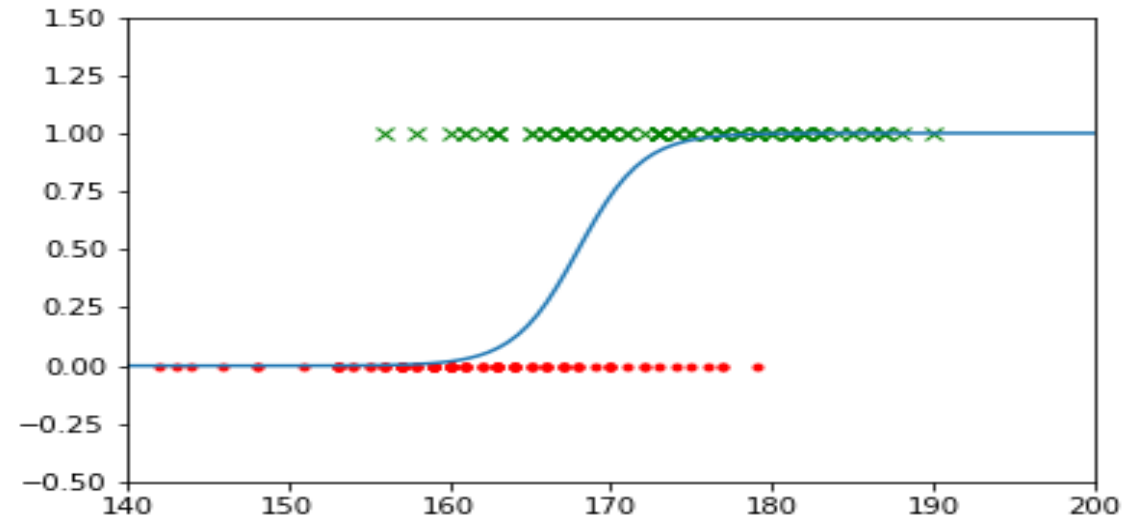
Supervised learning - Where are we?

	Classification	Regression
Decision tree	Lec.1 (simplified form)	
k Nearest Neighbors	Lec.5	
Perceptron	Lec.5	
Linear regression		Lec. 6
Logistic regression		
Neural networks		

Supervised learning - Where are we?

	Classification	Regression
Decision tree	Lec.1 (simplified form)	
k Nearest Neighbors	Lec.5	Possible
Perceptron	Lec.6	
Linear regression	today	Lec. 6
Logistic regression	today!	
Neural networks	Next week	

Logistic regression?

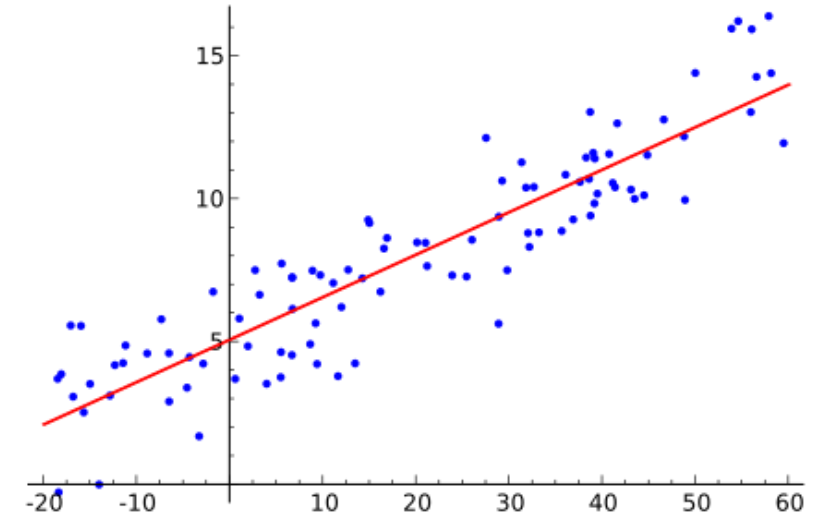
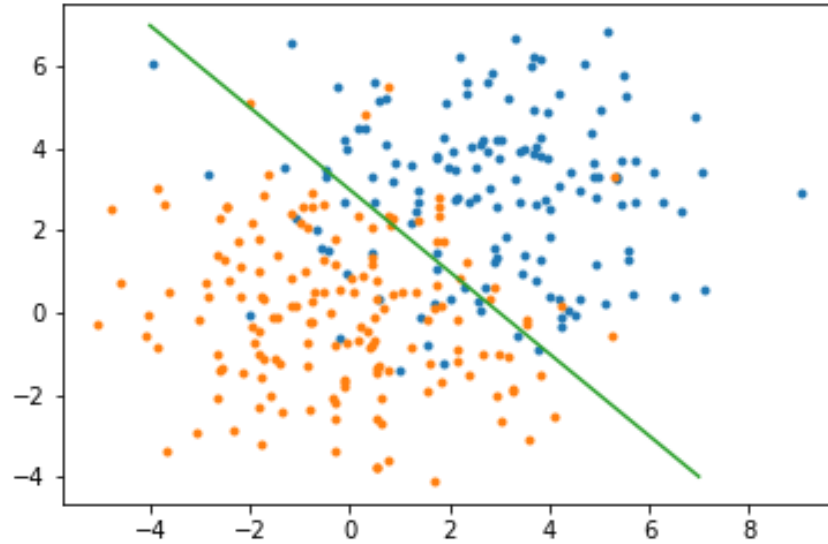


Interesting by itself

- A classifier
 - (not numerical regression)
- “Standard” (“best”) purely linear classifier
- (Not in Marsland)

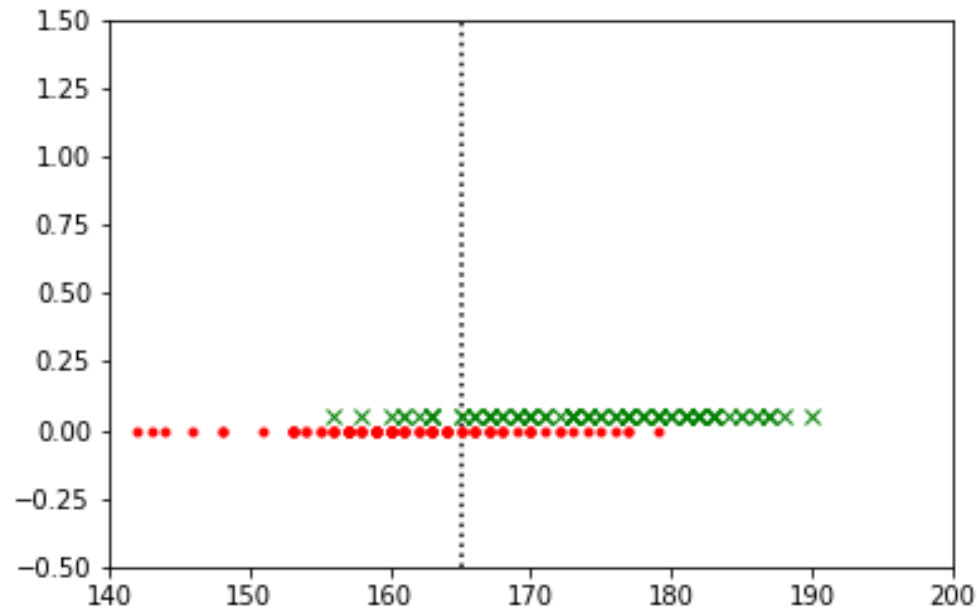
Useful tools for neural networks:

- The logistic function:
 - Its derivative
- Loss function
- Application of the chain rule for derivatives for gradient descent



	Linear Classifier	Linear regression
Number of input variable	Decision boundary	Prediction
One	Point	Line
Two	Line	Plane
Three	Plane	Hyper-plane
>3	Hyper-plane	
Update	Perceptron: $w_i = w_i - \eta(y - t)x_i$	$w_k = w_k - \eta \frac{2}{N} \sum_{j=1}^N ((t_j - y_j)(-x_{j,k}))$
Type of y, t	{0,1}	Real numbers

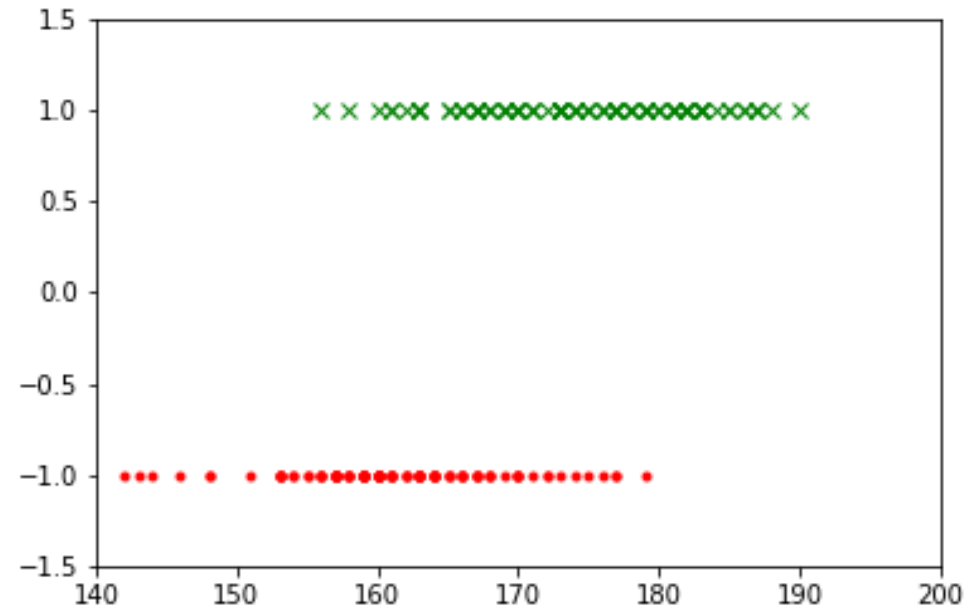
Example: predicting gender from height



- The decision boundary should be a number: c
- An observation, n , is classified
 - *male* if $height_n > c$
 - *female* otherwise
- How do we determine c ?

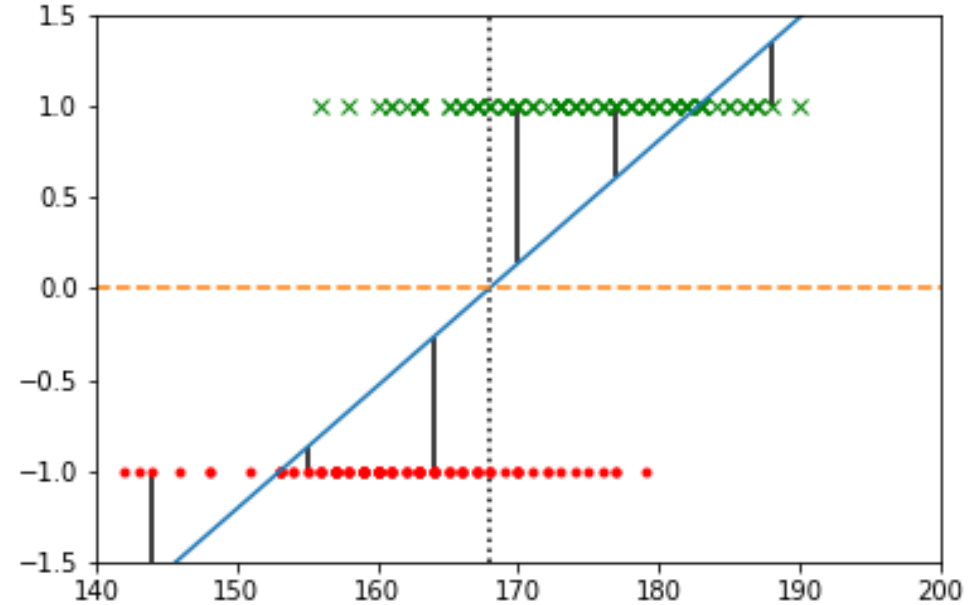
Linear regression as a classifier

1. Consider the prediction of classes as prediction of the two numbers 1, -1, resp.
2. Fit a linear regressor to these data (minimizing) MSE



Linear regression as a classifier

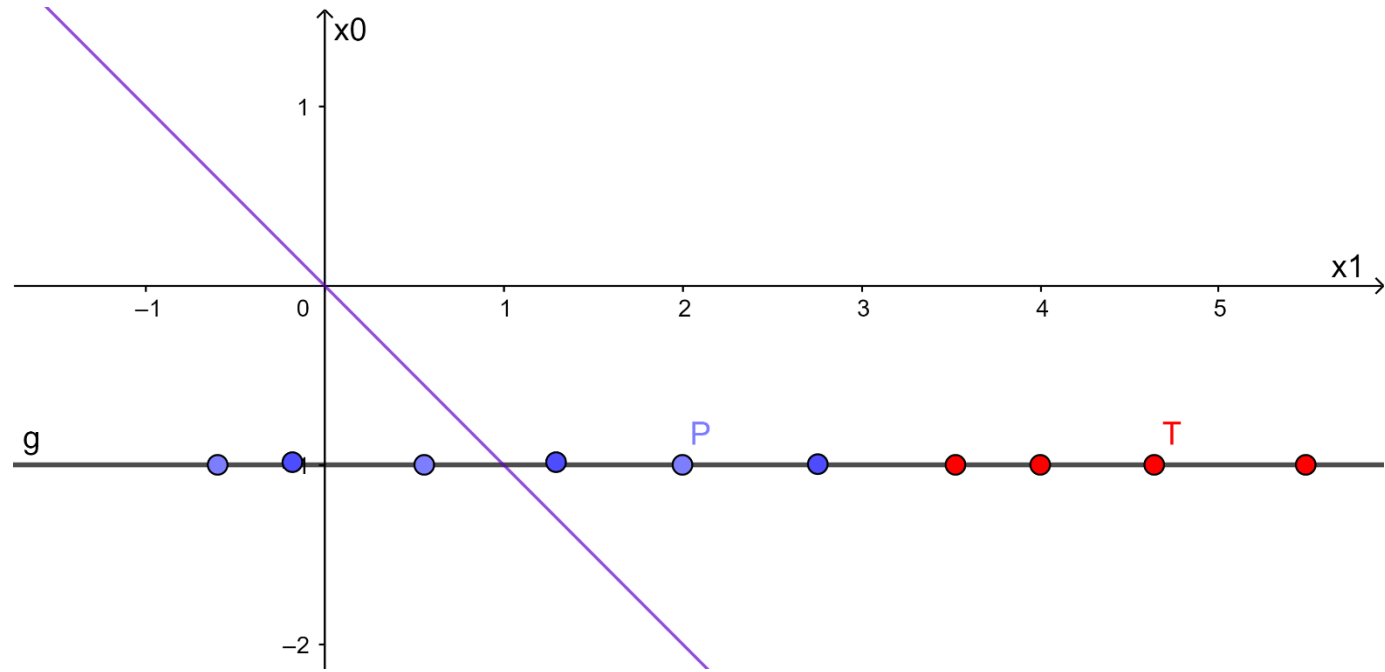
1. Consider the prediction of classes as prediction of the two numbers 1, -1, resp.
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Linear regression as a classifier

1. Consider the prediction of classes as prediction of the two numbers 1, -1, resp.
 2. Fit a linear regressor to these data (minimizing) MSE
 3. Predict
 - Positive class if $y > 0$ and
 - Negative class, otherwise otherwise
-
1. Consider the prediction of classes as prediction of the two numbers 1, -1, resp.
 2. Fit a linear regressor to these data (minimizing) MSE
 3. Predict
 - Positive class if $y > 0$ and
 - Negative class, otherwise otherwise
- Hence, decision boundary is dotted black line

Example

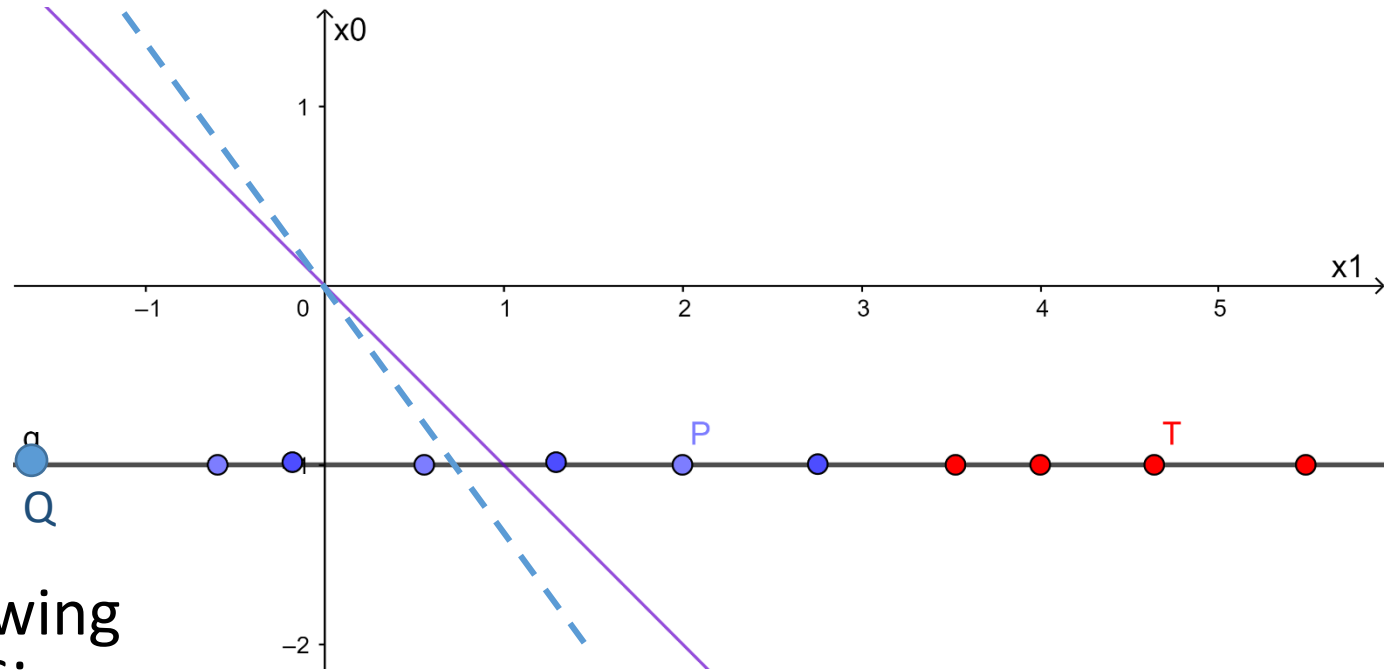


- Consider example from last week.
- Compare Lin.reg.-classifier to perceptron
- Assume stochastic gradient descent:
We update for one datapoint at a time

Example

- We are in the middle of training
- Learning rate: $\eta = 0.1$
- We have so far, the following weights for the decisions:
- Positive class provided
$$h = -w_0 + w_1 x_1 = 1 - x_1 > 0$$
 - i.e., $w_0 = -1$ and $w_1 = -1$

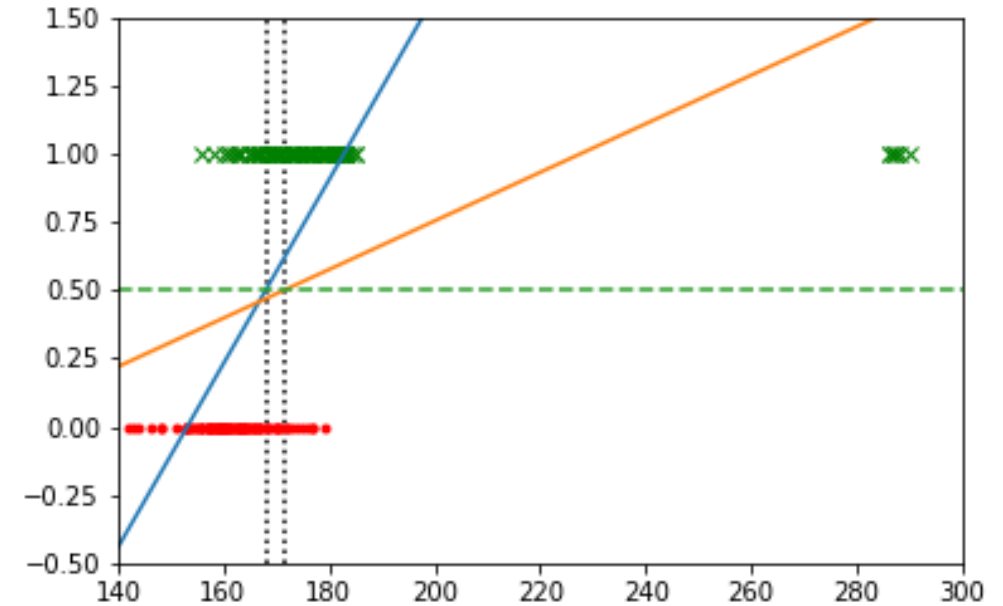
- Consider the point $Q=(-1, -2)$:
 - Correctly classified
 - Perceptron: Do nothing



- Lin.reg.classifier:
- $h(Q) = 1 - 1(-2) = 3$
 - $w_0 = w_0 - \eta(y - t)x_0 = -1 - 0.1(3 - 1)(-1) = -0.8$
 - $w_1 = w_1 - \eta(y - t)x_1 = -1 - 0.1(3 - 1)(-2) = -0.6$

Limitations

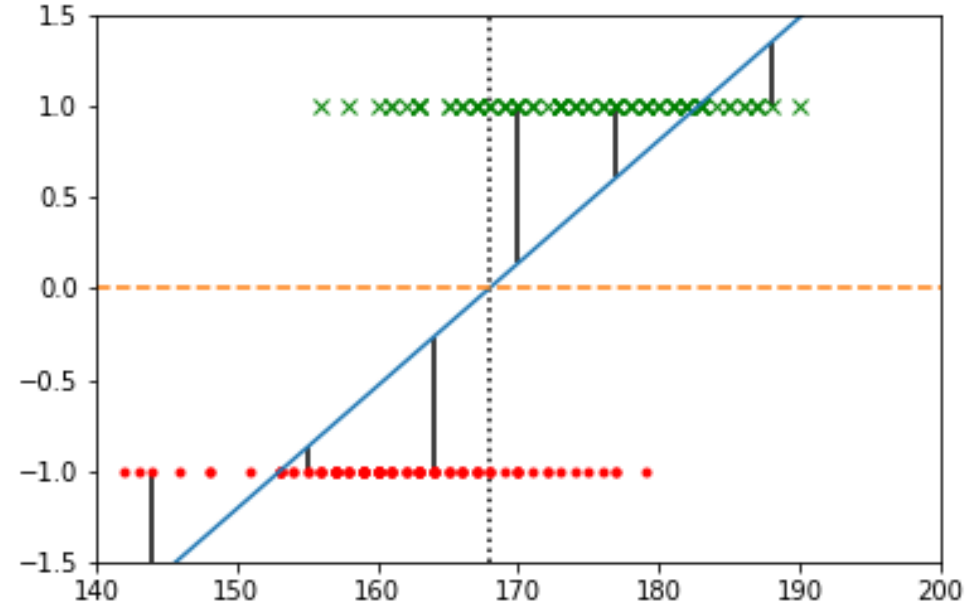
- For example
 - moving 7 (out of) 100 pos
100 steps to the right
 - the decision boundary is moved
 - from 168
 - to 171.5
 - the accuracy (on the 200 training set) goes
 - from 0.81
 - to 0.78
- Should these outliers have such an effect?



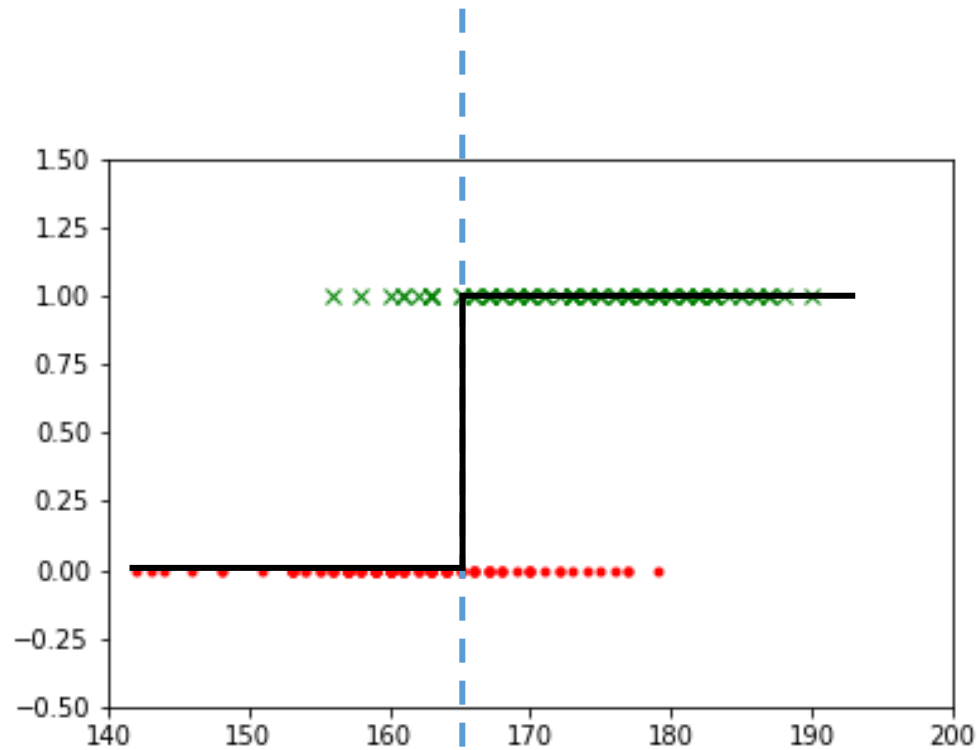
By the way:
We have here used 0 and 1 for the two classes.
This works equally fine.
Prediction: Positive class for $y > 0.5$

Linear regression as a classifier

- The MSE seems to punish correctly classified items too severely.



The “correct” decision boundary

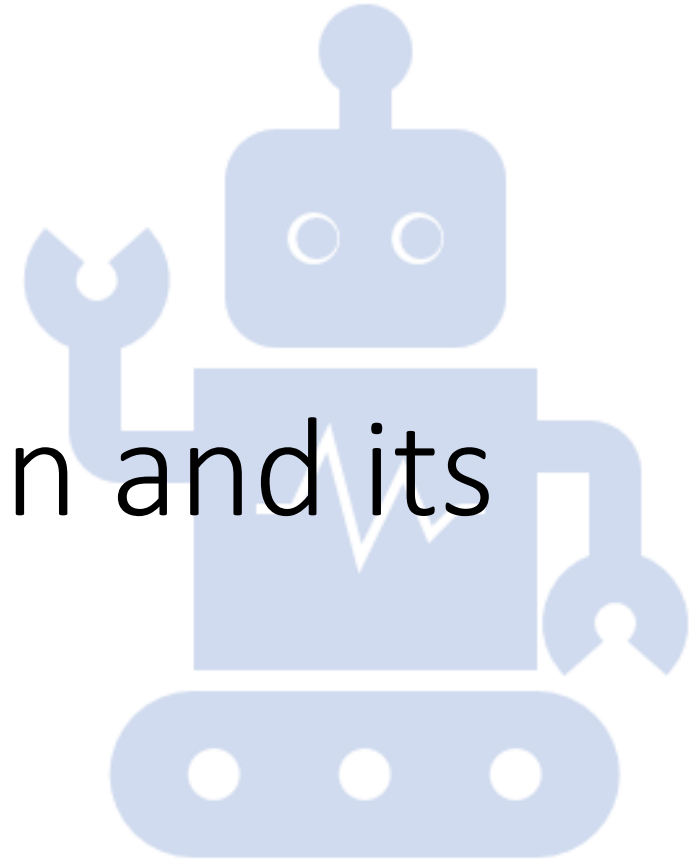


- The (Heaviside) step function
- But:
 - How do we find the best one?
 - Not a differentiable function

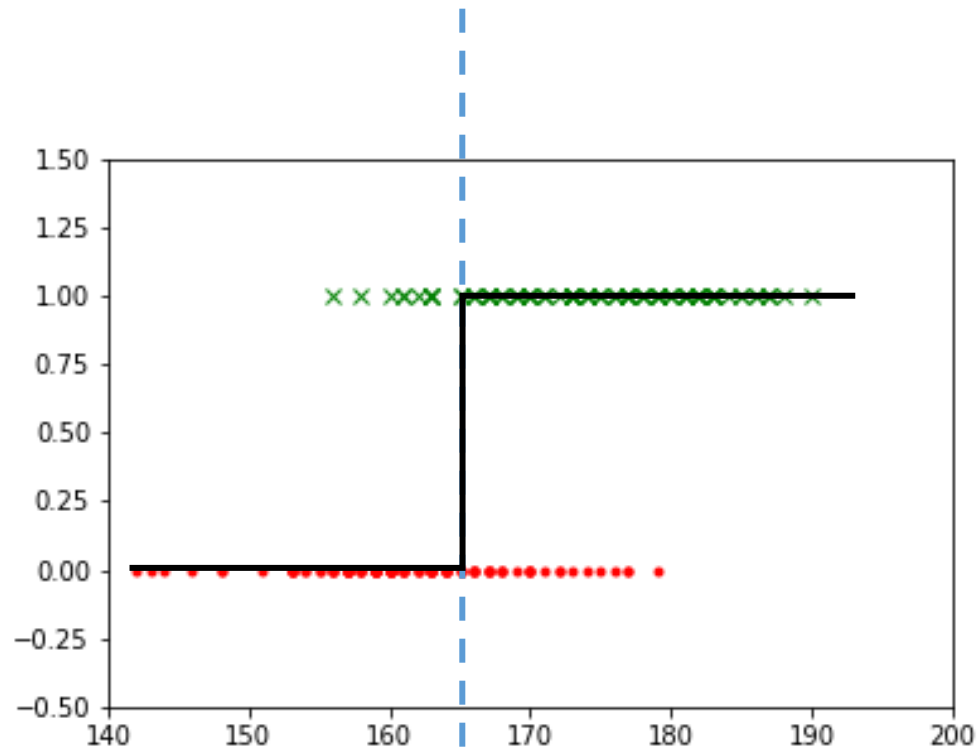


7.2 The Logistic Function and its Derivative

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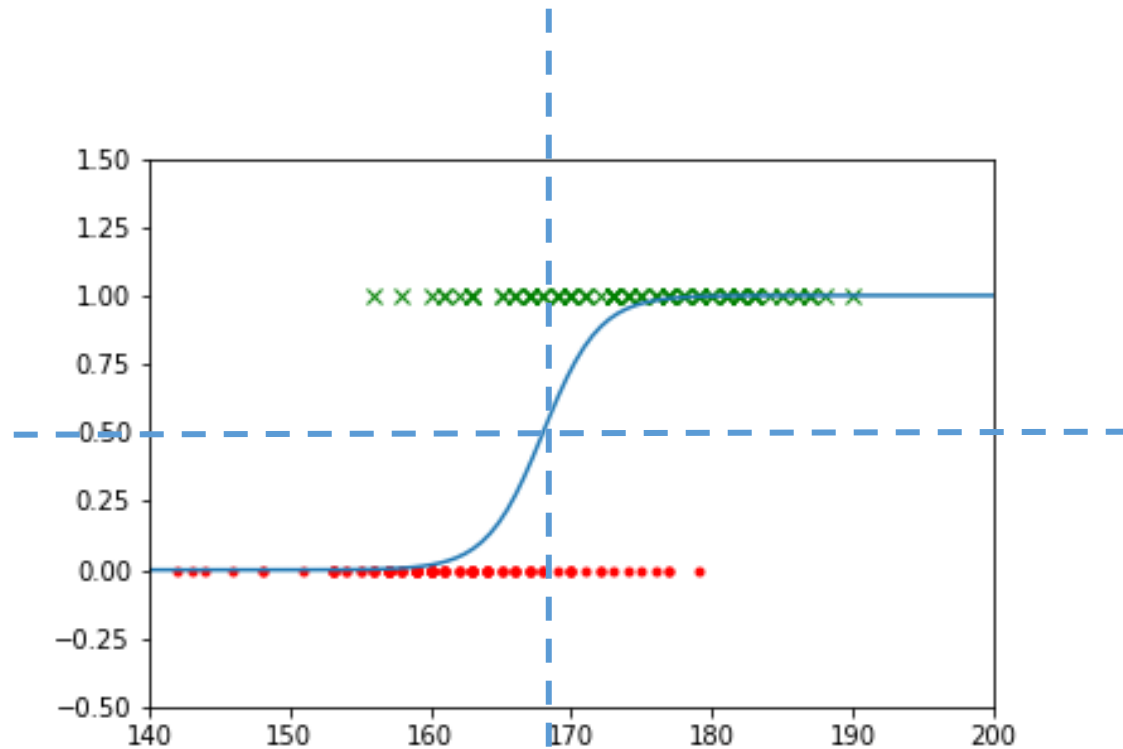


The “correct” decision boundary



- The (Heaviside) step function
- But:
 - How do we find the best one?
 - Not a differentiable function

The sigmoid curve



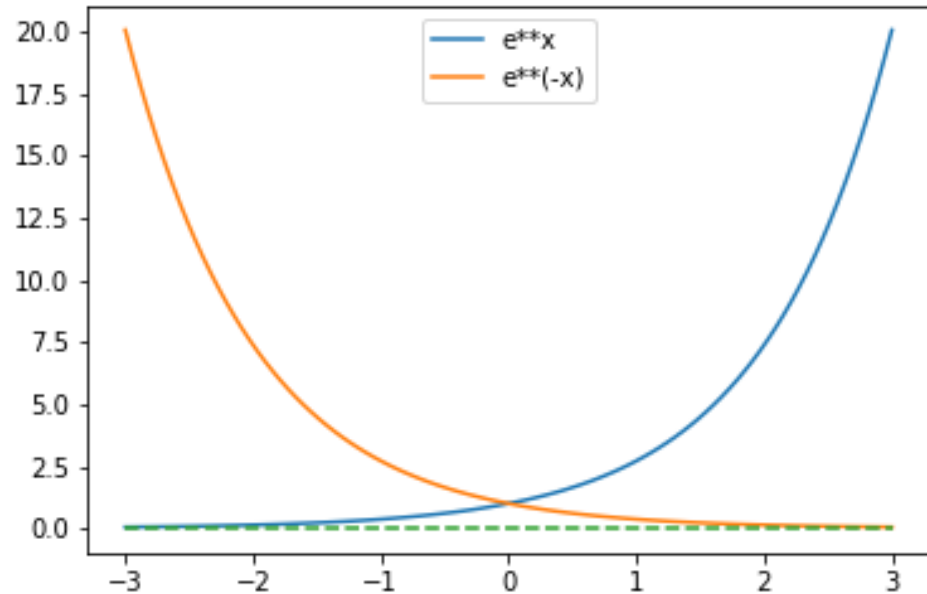
- An approximation to the ideal decision boundary
- Differentiable
 - Gradient descent
- Mistakes further from the decision boundary are punished harder

An observation, n , is classified

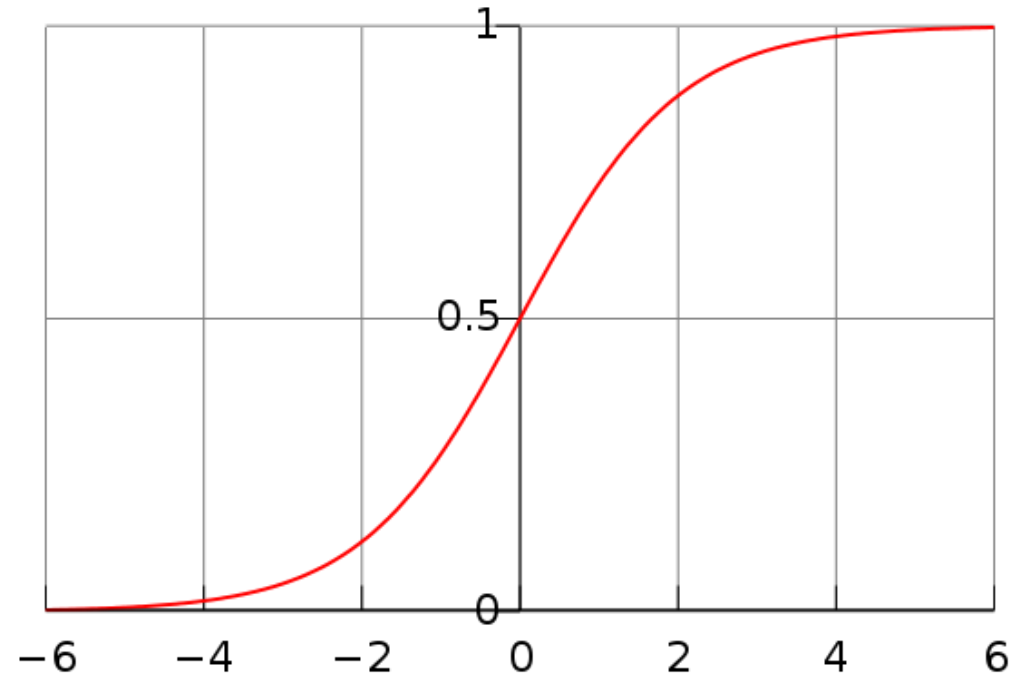
- *male* if $f(\text{height}_n) > 0.5$
- *female* otherwise

Exponential function - Logistic function

$$y = e^z$$

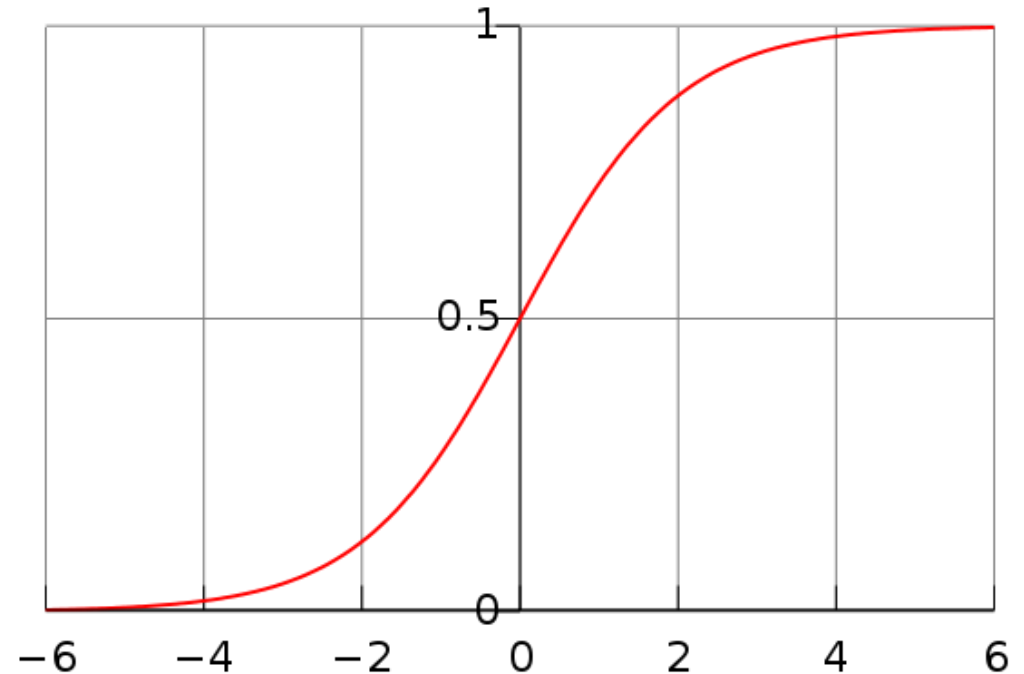


$$y = \frac{1}{1 + e^{-z}} = \frac{e^z}{e^z + 1}$$



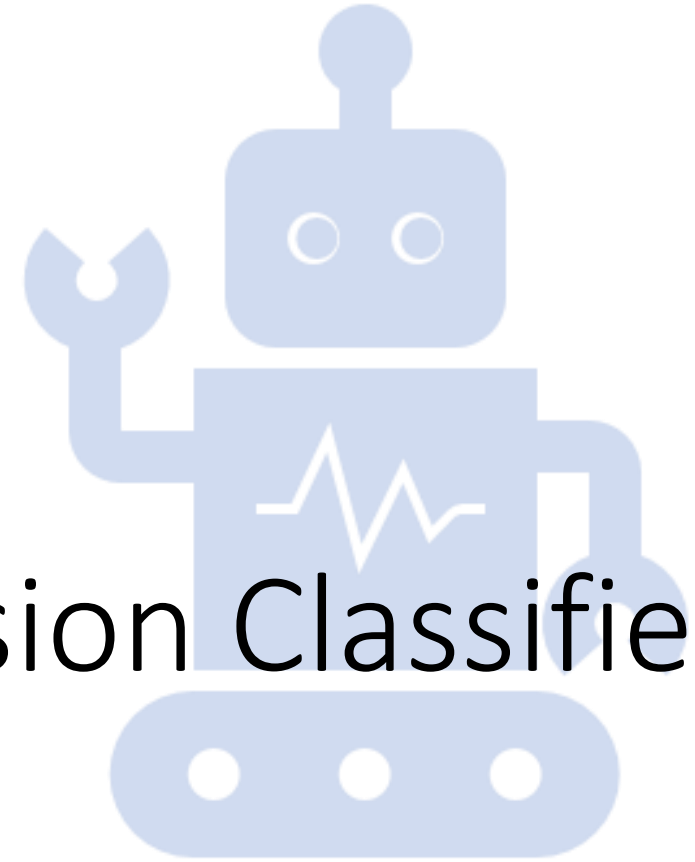
The logistic function

- $y = \frac{1}{1+e^{-z}} = \frac{e^z}{e^z+1}$
- A sigmoid curve
 - Other functions also make sigmoid curves e.g., $y = \tanh(z)$
- Maps $(-\infty, \infty)$ to $(0,1)$
- Monotone
- Can be used for transforming numeric values into probabilities



The derivative of the logistic function

- $y = f(x) = \frac{1}{1+e^{-x}}$
- This has the form $y = g(h(x))$
where $g(z) = \frac{1}{z}$ and $z = h(x) = 1 + e^{-x}$
- Hence $f'(x) = g'(z)h'(x) = \frac{-1}{(1+e^{-x})^2} (-e^{-x}) =$
- $\frac{e^{-x}+1-1}{(1+e^{-x})^2} = \frac{e^{-x}+1}{(1+e^{-x})^2} - \frac{1}{(1+e^{-x})^2} = y - y^2 = y(1 - y)$
- We will use this also in the multi-layer neural networks



7.3 The Logistic Regression Classifier

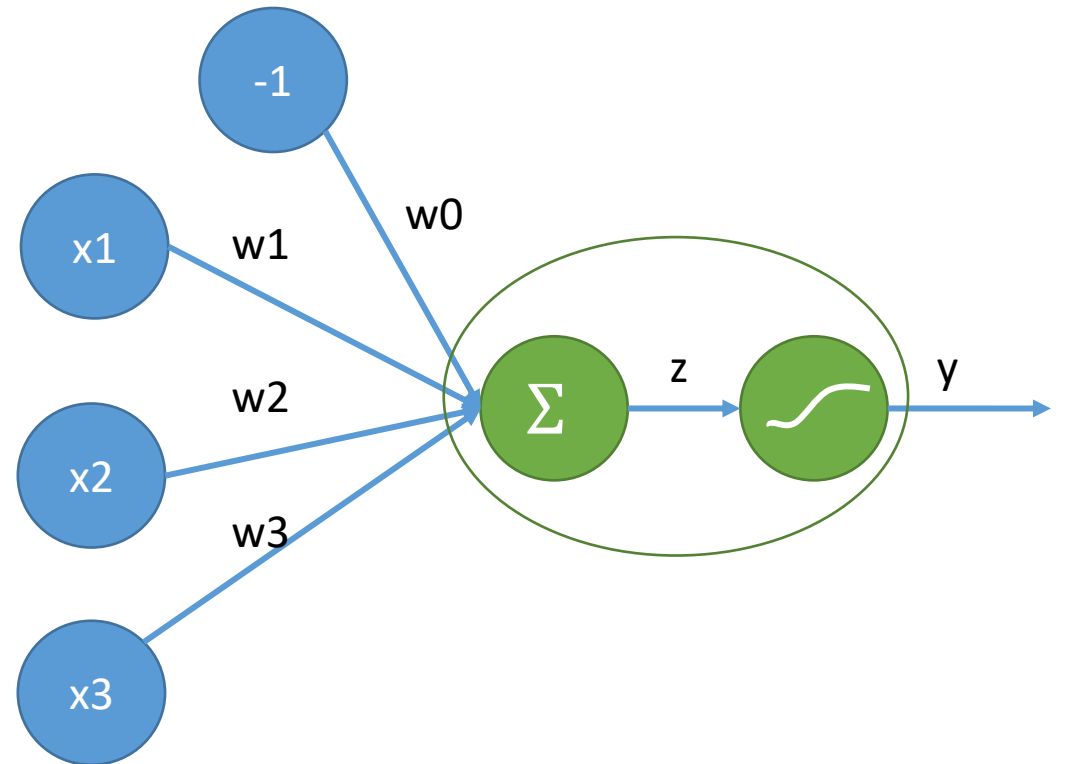
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Logistic Regression:

- First sum of weighted inputs :
- $z = \sum_{i=0}^m w_i x_i = \mathbf{w} \cdot \mathbf{x}$
- Apply the logistic function σ to this sum

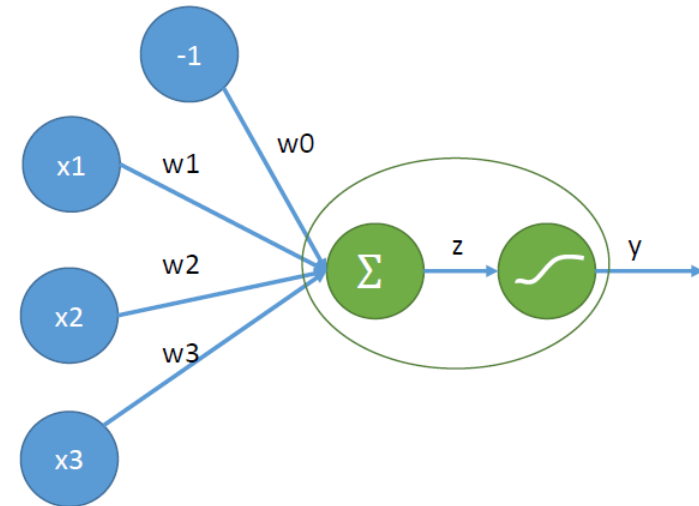
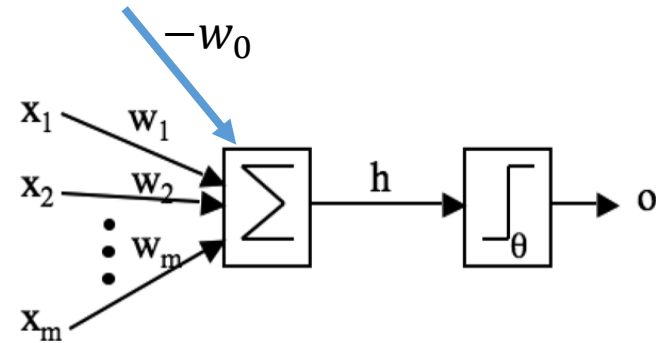
$$y = \sigma(z) = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}}$$

- For $\mathbf{x} = \vec{x}$ **predict**
 - as the positive class if $y > 0.5$,
 - otherwise, the negative class

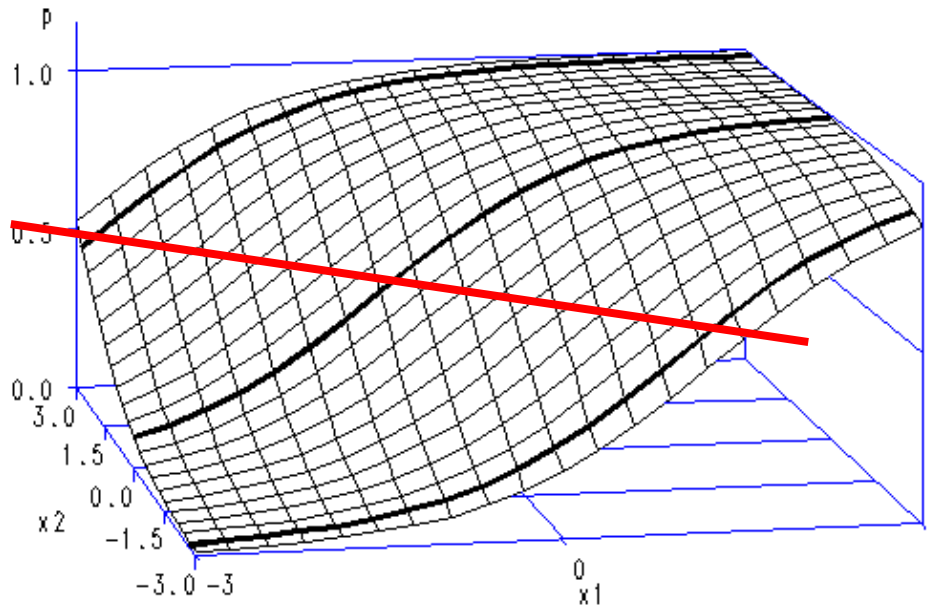


Comparison: activation function

- Perceptron: step function
- Linear regression: identity
- Logistic regression: the logistic function



With two features



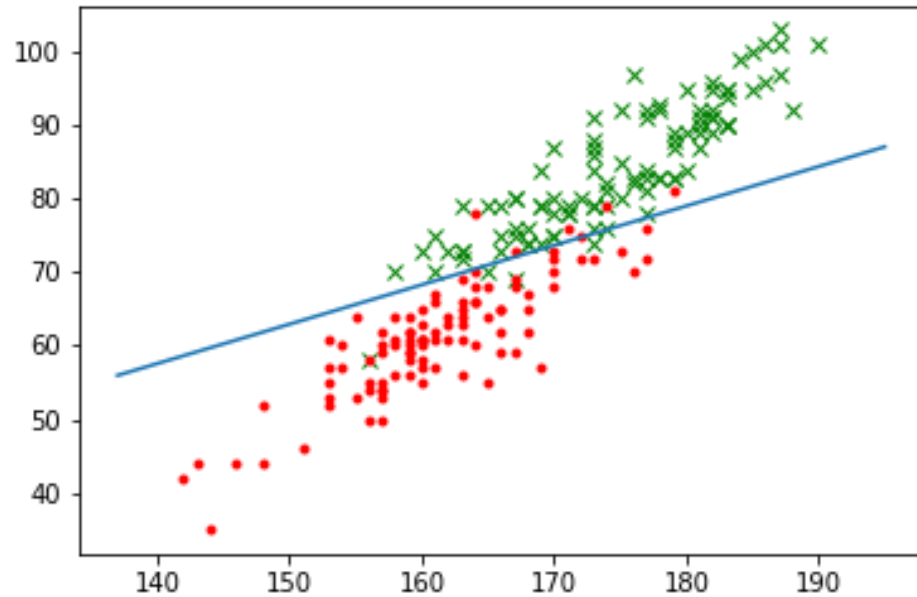
From IDRE, UCLA

- Two features: x_1, x_2
- Apply weights: w_0, w_1, w_2
- Let $y = -w_0 + w_1x_1 + w_2x_2$
- Apply the logistic function, σ , and check whether

$$\bullet \sigma(y) = \frac{1}{1+e^{-y}} > 0.5$$

Geometrically: Folding a plane along a sigmoid
The decision boundary is the intersection of
this surface and the plane $p = \sigma(y) = 0.5$:
This turns out to be a straight line

Example with two features



- Example:
 - Heights and weights
 - Acc.: = 0.95
- Blue line = decision boundary
 - Points above it gets a value > 0.5

Understanding logistic regression 1

The following 3 slides attempt to give you an understanding of logistic regressions models.

- The model is probability-based
- There are two classes $t=1$, $t=0$
- For an observation $\mathbf{x} = \vec{x}$, we wonder:
- *How probable is it that this \vec{x} belongs to class 1, and how probable is it that it belongs to class 0?*
- i.e., what are $P(t = 1|\vec{x})$ and $P(t = 0|\vec{x})$? Which is largest?

Understanding logistic regression 2

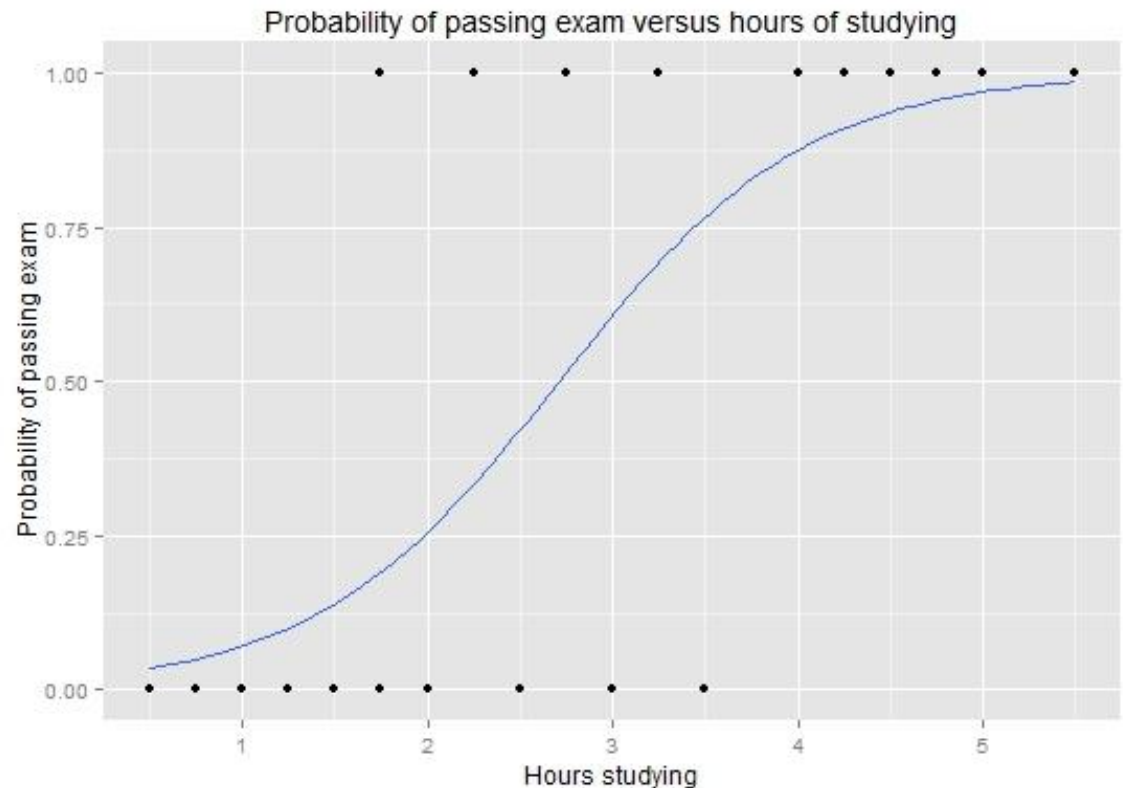
- What are $P(t = 1|\vec{x})$ and $P(t = 0|\vec{x})$? Which is largest?
- Consider the **odds**: $\frac{P(t=1|\vec{x})}{P(t=0|\vec{x})} = \frac{P(t=1|\vec{x})}{1-P(t=1|\vec{x})}$
 - If this is >1 , \vec{x} most probably belongs to $t=1$, otherwise $t=0$
 - The odds varies between 0 and infinity
- Take the logarithm of this, $\log \frac{P(t=1|\vec{x})}{1-P(t=1|\vec{x})}$
 - If this is >0 , \vec{x} most probably belongs to $t=1$
 - This varies between minus infinity and plus infinity

Understanding logistic regression 3

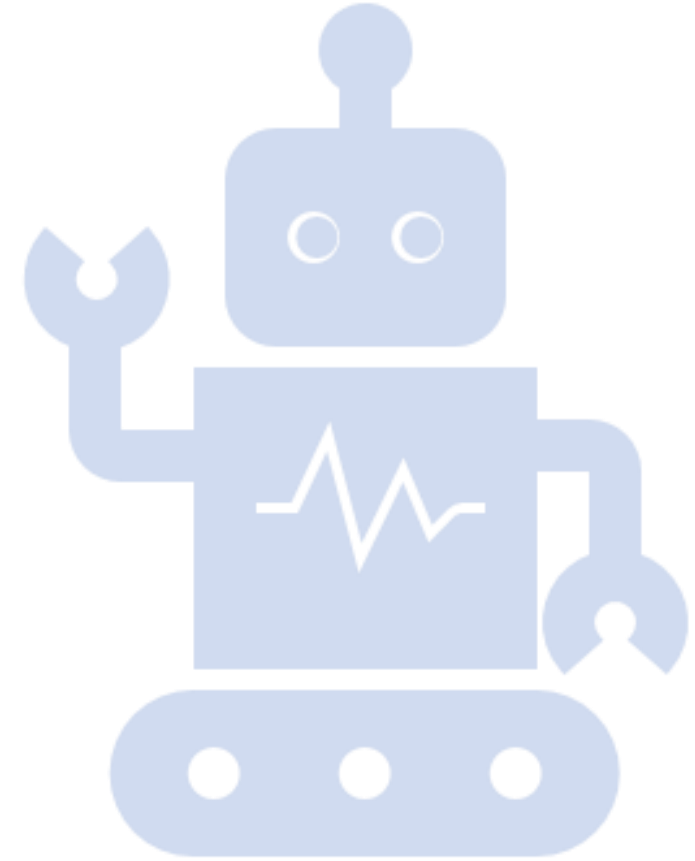
- $\log \frac{P(t=1|\vec{x})}{1-P(t=1|\vec{x})} > 0$?
- Try to find a linear expression for this, $\log \left(\frac{P(t=1|\vec{x})}{1-P(t=1|\vec{x})} \right) = \vec{w} \cdot \vec{x} > 0$
- Given such a linear expression, then
 - $\frac{P(t=1|\vec{x})}{1-P(t=1|\vec{x})} = e^{\vec{w} \cdot \vec{x}}$
- Solving this with respect to $P(t = 1|\vec{x})$ yields
 - $P(t = 1|\vec{x}) = \frac{e^{\vec{w} \cdot \vec{x}}}{1+e^{\vec{w} \cdot \vec{x}}} = \frac{1}{1+e^{-\vec{w} \cdot \vec{x}}}$

A probabilistic classifier

- The logistic regression will ascribe a probability to all instances for the class $t=1$ (and for $t=0$)
- We turn it into a classifier by ascribing class $t=1$ if
$$P(t = 1|\vec{x}) > 0.5$$
- We could also choose other cut-offs, e.g., if the classes are not equally important.



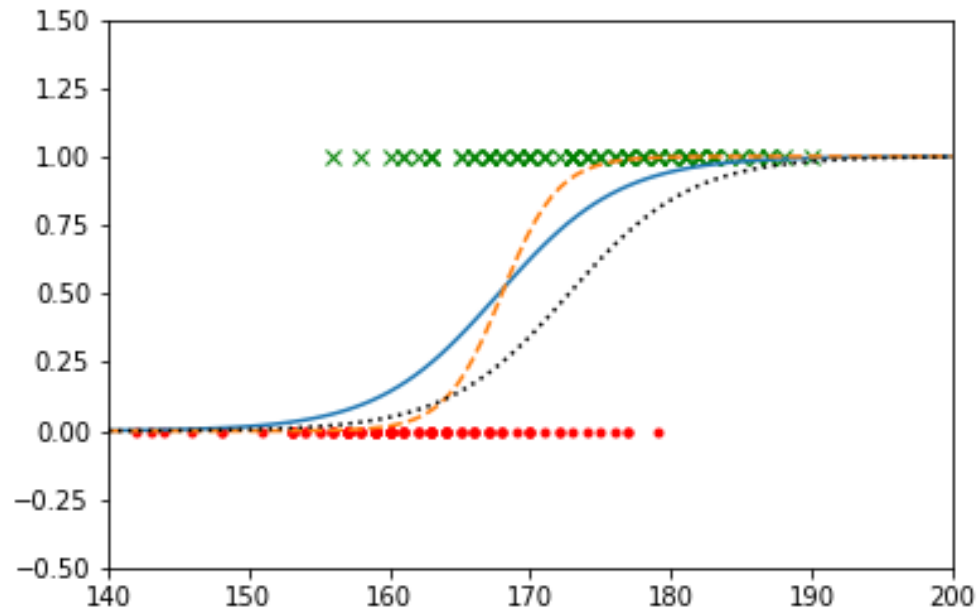
source: Wikipedia



7.4 Cross-Entropy Loss

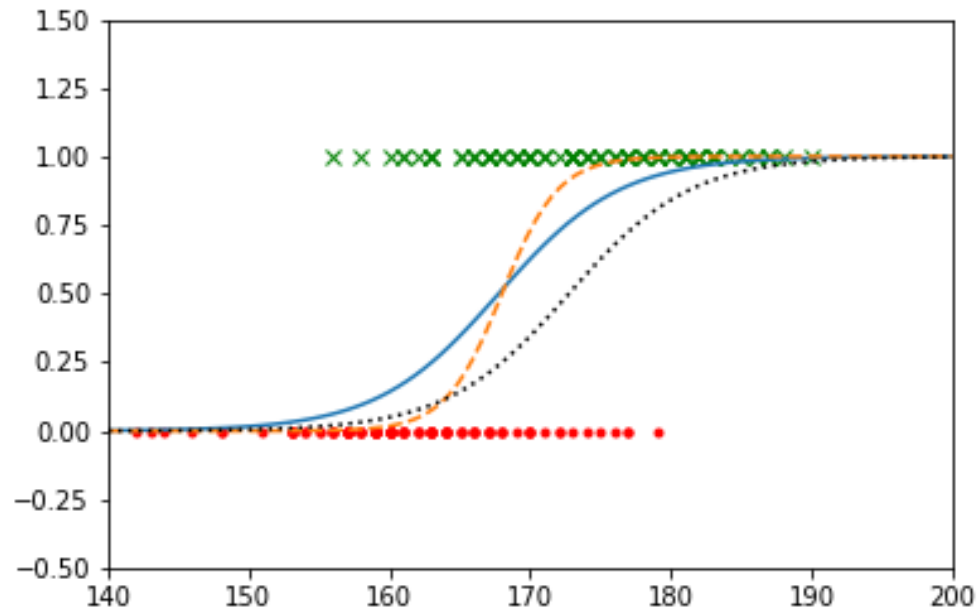
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How to find the best curve?



- What are the best choices of a and b in $\frac{1}{1+e^{-(ax+b)}}$?
- Geometrically a and b determine the
 - Midpoint (b)
 - Steepness (a)
- of the curve
- What are the best choices of \vec{w}
$$y = P(t = 1|\vec{x}) = \frac{1}{1+e^{-\vec{w}\cdot\vec{x}}}$$

Learning in the logistic regression model



- A training instance consists of
 - a feature vector \vec{x}
 - a label (class), t , which is 1 or 0.
- With a set of weights, \vec{w} , the classifier will assign
 - $y = P(t = 1|\vec{x}) = \frac{1}{1+e^{-\vec{w}\cdot\vec{x}}}$ to this training instance \vec{x}
 - where $P(t = 0|\vec{x}) = 1 - y$
- Goal: find \vec{w} that maximize $P(t|\vec{x})$ of all training inst.s (\vec{x}, t)

Loss function

35

- In machine learning we decide on an **objective** for the training.
- We can do that in terms of a **loss function**.
- The goal of the training is to minimize the loss function.
- Example: linear regression
 - Loss: Mean Square Error
- We can choose between various loss functions.
- The choice is partly determined by the learner.
- For logistic regression we choose (simplified) **cross-entropy loss**

Footnote: Notation

- I observe that I haven't been consequent in notation
- I fluctuate between boldface \mathbf{x} and non-bold with an arrow \vec{x} . There are no (intended) differences between the two, $\mathbf{x} = \vec{x}$
- I have also fluctuated between x_j and $\vec{x}^{(j)}$ for vector number j in the input set. Again, the two ways of writing amount to the same.

The money game

- I will give you 10 multiple-choice questions. You must answer all.
- I give you a million NOK before the game.
- In each round, you must bet your remaining money on the alternatives. Say there are 3 answers in the first round. You could bet any of the following, e.g.

	Your bet			You keep		
	Answer A	Answer B	Answer C	If A correct	If B correct	If C correct
Strategy 1	1,000,000	0	0	1,000,000	0	0
Strategy 2	400,000	300,000	300,000	400,000	300,000	300,000
Strategy 3	800,000	150,000	50,000	800,000	150,000	50,000

- You proceed to the next round with the money you keep.
- What would be the best strategy?

Cross-entropy loss

- The underlying idea is that we want to maximize the joint probability of all the predictions we make
 - $\prod_{i=1}^N P(t^{(i)} | \vec{x}^{(i)})$, over all the training data $i = 1, 2, \dots, N$
 - (since the training data are independent)
- This is the same as maximizing
 - $\log \prod_{i=1}^N P(t^{(i)} | \vec{x}^{(i)}) = \sum_{i=1}^N \log P(t^{(i)} | \vec{x}^{(i)})$
- This is the same as minimizing
 - $L_{CE}(\vec{w}) = -\log \prod_{i=1}^N P(t^{(i)} | \vec{x}^{(i)}) = \sum_{i=1}^N -\log P(t^{(i)} | \vec{x}^{(i)})$
 - Which is an instance of what is called the cross-entropy loss

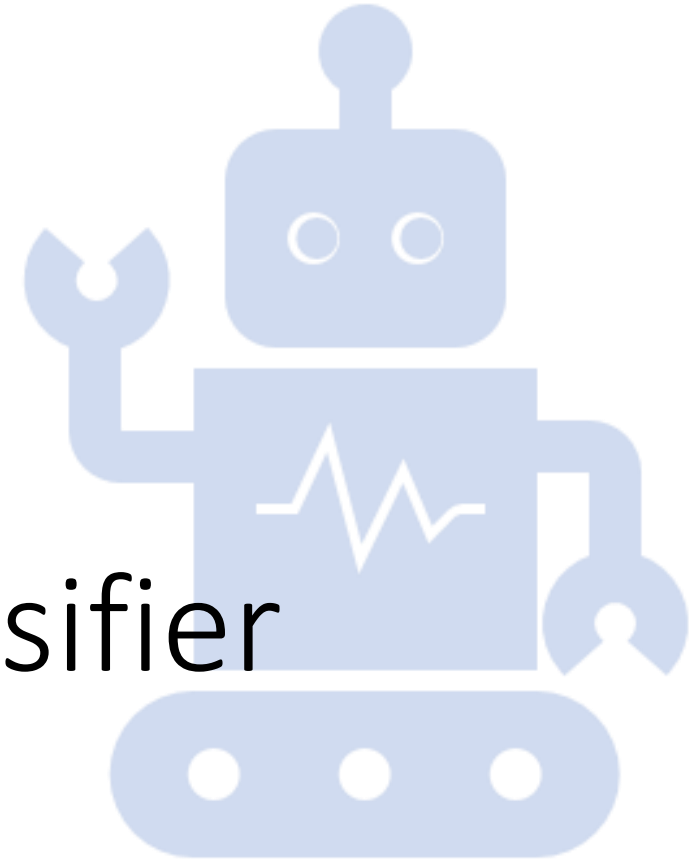
More on cross-entropy loss

- When $t = 1$, $P(t | \vec{x}) = y = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}}$
- When $t = 0$, $P(t | \vec{x}) = 1 - y$
- Since
 - $y^t = y$ when $t = 1$
 - $y^t = 1$ when $t = 0$
 - $(1 - y)^{(1-t)} = 1$ when $t = 1$
 - $(1 - y)^{(1-t)} = (1 - y)$ when $t = 0$
- $P(t|\vec{x}) = y^t(1 - y)^{(1-t)}$, whether $t = 1$ or $t = 0$



7.5 Training the Logistic Regression Classifier

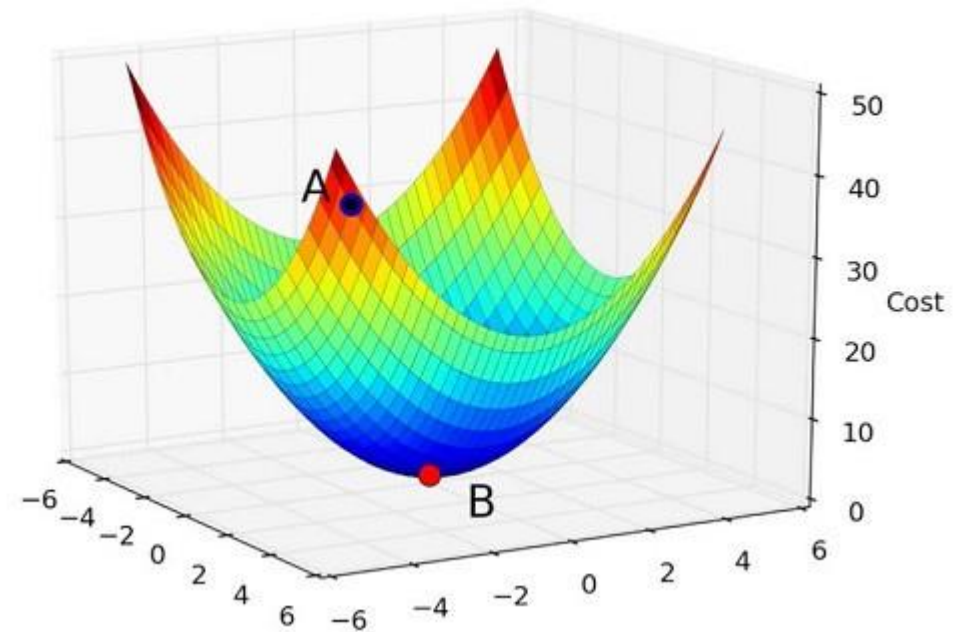
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Gradient descent

41

- The loss function tells us which model is best.
- How do we find it?
- No closed-form solution, i.e., formula as there are for linear regression,
- Good news:
 - The log-loss function is convex: you are not stuck in local minima
 - We know which way to go



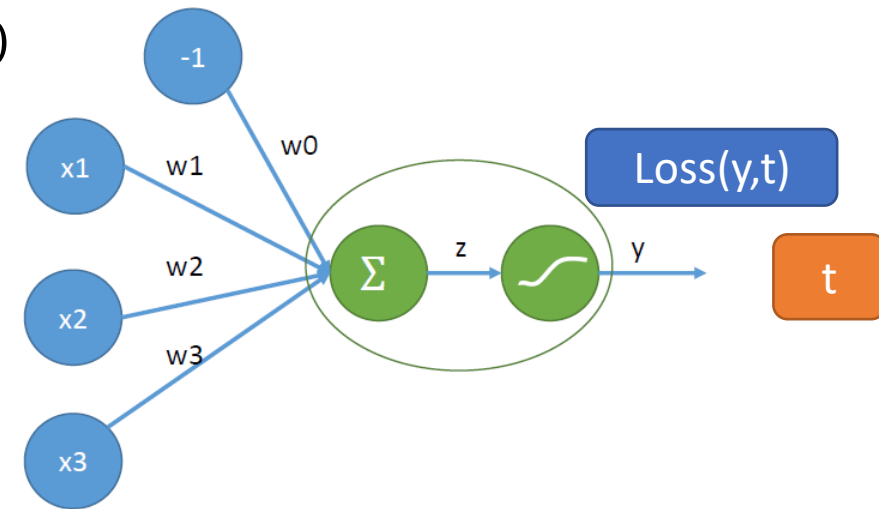
The gradient

- We have

- $L_{CE}(\vec{w}) = -\log \prod_{i=1}^N P(t^{(i)} | \vec{x}^{(i)}) = \sum_{i=1}^N -\log P(t^{(i)} | \vec{x}^{(i)})$
- $P(t | \vec{x}) = y^t (1 - y)^{(1-t)}$
- $y = \sigma(\vec{w} \cdot \vec{x}) = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}}$

- We shall find

- $\frac{\partial}{\partial w_j} L_{CE}(\vec{w})$ for each w_j
- since $\frac{\partial}{\partial w_j} L_{CE}(\vec{w}) = \sum_{i=1}^N -\frac{\partial}{\partial w_j} \log P(t^{(i)} | \vec{x}^{(i)})$
- we can consider what this looks like for one pair $(\vec{x}^{(i)}, t^{(i)})$ at a time
- $-\frac{\partial}{\partial w_i} \log P(t | \vec{x}) = -\frac{\partial}{\partial w_i} \left(\log(y^t (1 - y)^{(1-t)}) \right) =$
 $-\frac{\partial}{\partial w_i} (t \log(y) + (1 - t) \log(1 - y))$



Derivative: the chain rule

- We shall find

- $-\frac{\partial}{\partial w_i} \log P(t|\vec{x}) = -\frac{\partial}{\partial w_i} (t \log(y) + (1-t)\log(1-y))$

- $= -\frac{\partial}{\partial y} (t \log(y) + (1-t)\log(1-y)) \left(\frac{\partial}{\partial w_i} y \right)$ by the chain rule for derivatives

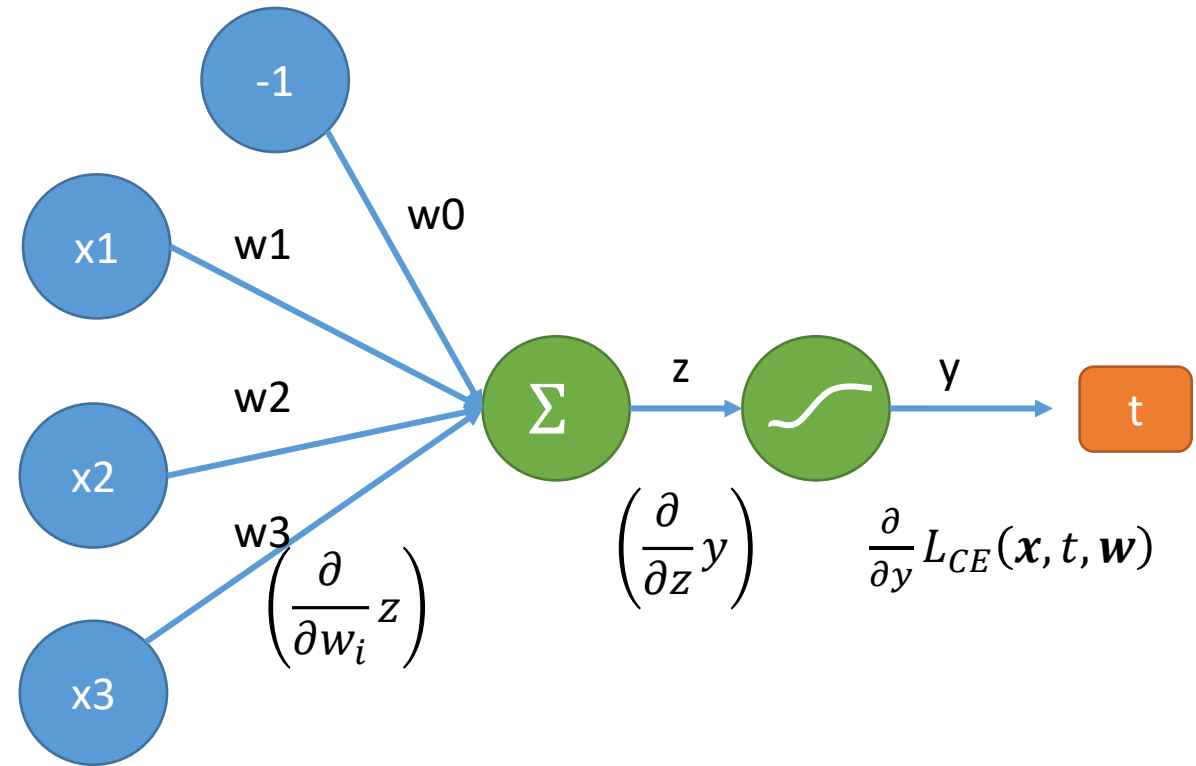
- $\frac{\partial}{\partial y} (t \log(y) + (1-t)\log(1-y)) = \frac{t}{y} - \frac{(1-t)}{(1-y)} = \frac{t(1-y)-y(1-t)}{y(1-y)} = \frac{(t-y)}{y(1-y)}$

The derivative of the logistic function

- $y = \sigma(\vec{w} \cdot \vec{x}) = \frac{1}{1+e^{-\vec{w} \cdot \vec{x}}} = \frac{1}{1+e^{-z}}$, where $z = \vec{w} \cdot \vec{x}$
- $\frac{\partial}{\partial w_i} y = \left(\frac{\partial}{\partial z} y\right) \left(\frac{\partial}{\partial w_i} z\right)$
- $\frac{\partial}{\partial z} y = y(1 - y)$ (the logistic function)
- $\frac{\partial}{\partial w_i} z = x_i$
- $\frac{\partial}{\partial w_i} y = y(1 - y)x_i$

Putting it together graphically

- $\frac{\partial}{\partial w_i} L_{CE}(\mathbf{x}, t, \mathbf{w}) =$
- $\frac{\partial}{\partial y} L_{CE}(\mathbf{x}, t, \mathbf{w}) \left(\frac{\partial}{\partial z} y \right) \left(\frac{\partial}{\partial w_i} z \right)$



Putting it all together

- $\frac{\partial}{\partial w_i} L_{CE}(\mathbf{x}, t, \mathbf{w}) = -\frac{\partial}{\partial w_i} \log P(t|\vec{x}) = -\frac{\partial}{\partial w_i} (t \log(y) + (1-t)\log(1-y))$

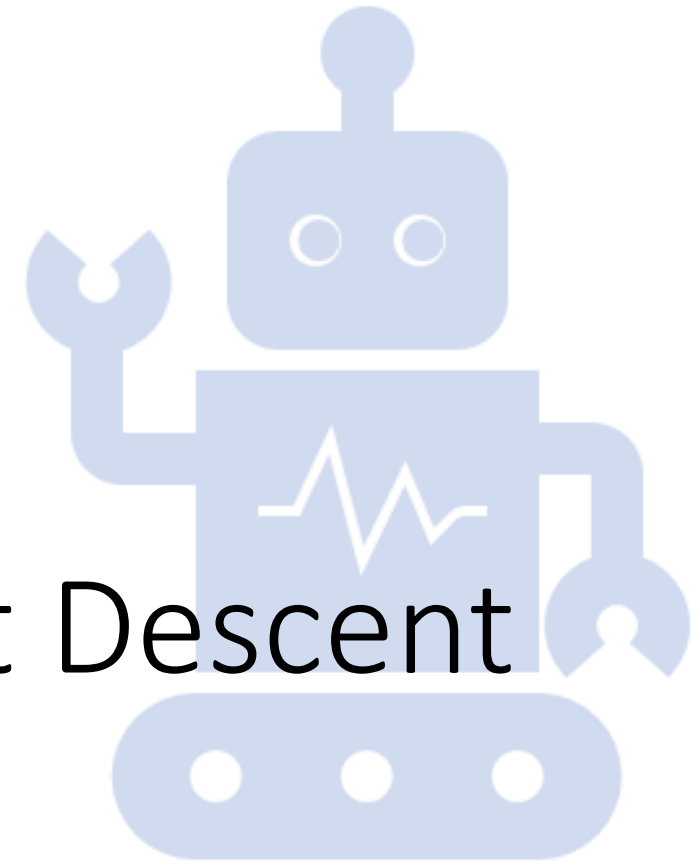
- $= -\frac{\partial}{\partial y} (t \log(y) + (1-t)\log(1-y)) \left(\frac{\partial}{\partial w_i} y \right)$

- $= -\frac{(t-y)}{y(1-y)} y(1-y)x_i = -(t-y)x_i$

- A long journey – but the result is simple

- Adding together (matrix multiplication) for all the training data yields the gradient

- $(\nabla f)_i = \frac{\partial}{\partial w_i} L_{CE}(X, T, \mathbf{w}) = \sum_{j=1}^N -(t_j - y_j)x_{j,i}$



7.6 Variants of Gradient Descent

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Variants of gradient descent

Batch training:

- Calculate the loss for the whole training set, and the gradient for this
- Make one move in the correct direction
- Repeat (an epoch)
- Can be slow

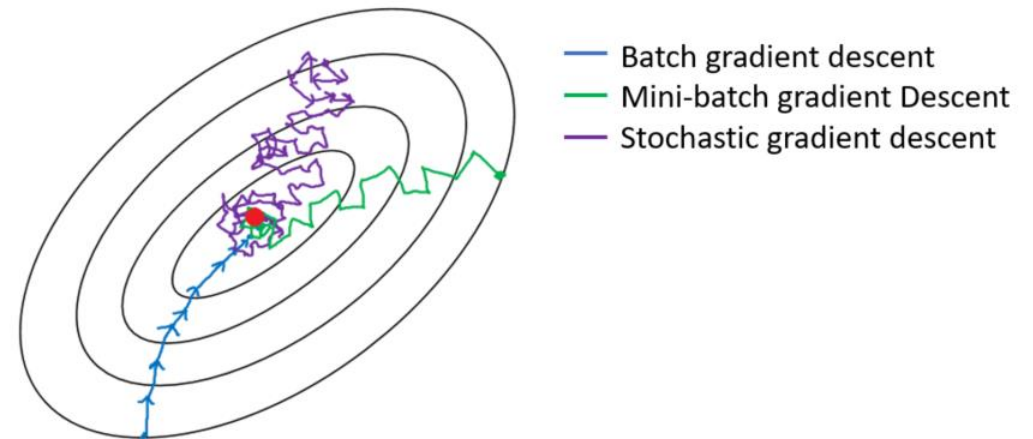
Stochastic gradient descent:

- Pick one item
- Calculate the loss for this item
- Calculate the gradient for this item and move in the opposite direction
- Each move does not have to be in towards the direction of the gradient for the whole set.
- But the overall effect may be good
- Can be faster

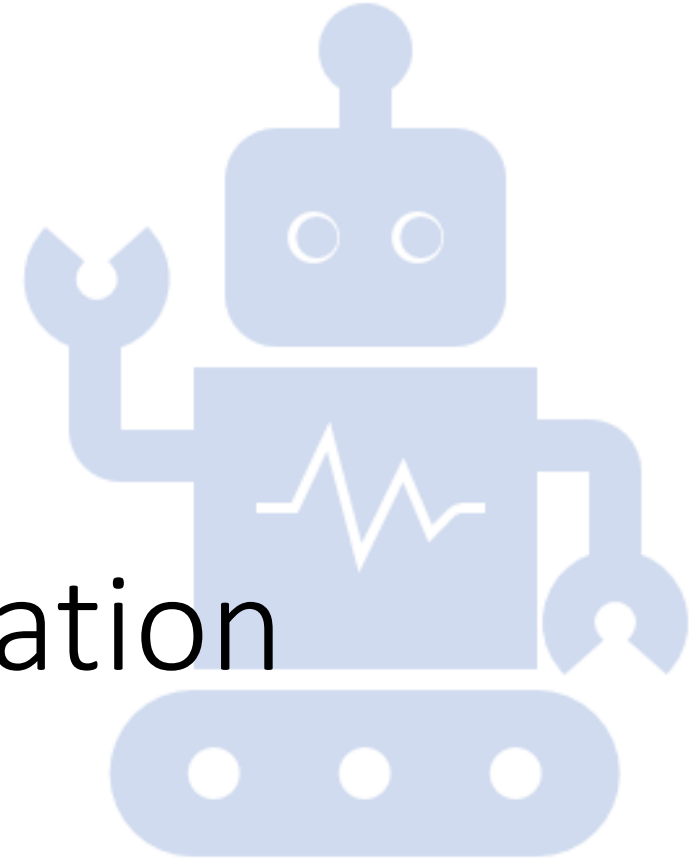
Variants of gradient descent

Mini-batch training:

- Pick a subset of the training set of a certain size
- Calculate the loss for this subset
- Make one move in the direction opposite of this gradient
- Repeat (an epoch)
- A good compromise between the two extremes
- (The other two are subcases of this)



<https://suniljangirblog.wordpress.com/2018/12/13/variants-of-gradient-descent/>



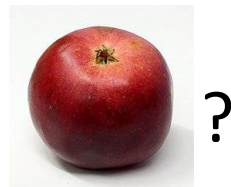
7.7 Multi-Class Classification

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Multi-class classification

Classification

- Assign a label (class) from a finite set of labels to an observation



- So far, many algorithms and examples have been binary: *yes-no, 1-0*
- But many classification tasks are multi-class:
 - To each observation x choose one label from a finite set T
- What is different?

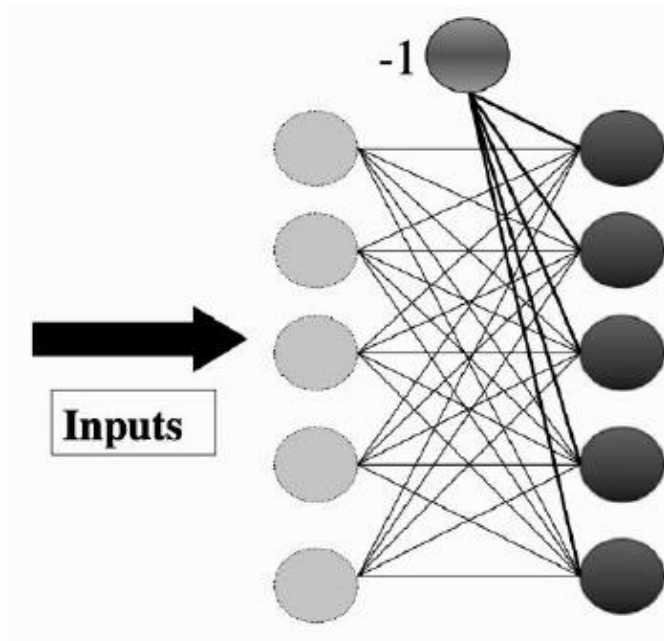
1-of-N or "one hot encoding"

- The labels might be categorical:
 - 'apple', 'tomato', 'dog', 'horse'
- The algorithms demand numerical attributes.
- First attempt
 - 'apple' = 1
 - 'tomato' = 2
 - 'dog' = 3
 - etc.
- Why isn't this a good idea?
- Better:
 - 'apple' = (1, 0, 0, 0, 0, 0)
 - 'tomato' = (0, 1, 0, 0, 0, 0)
 - 'dog' = (0, 0, 1, 0, 0, 0)
 - etc.
- Both the target and the predicted value are vectors.

One vs. rest

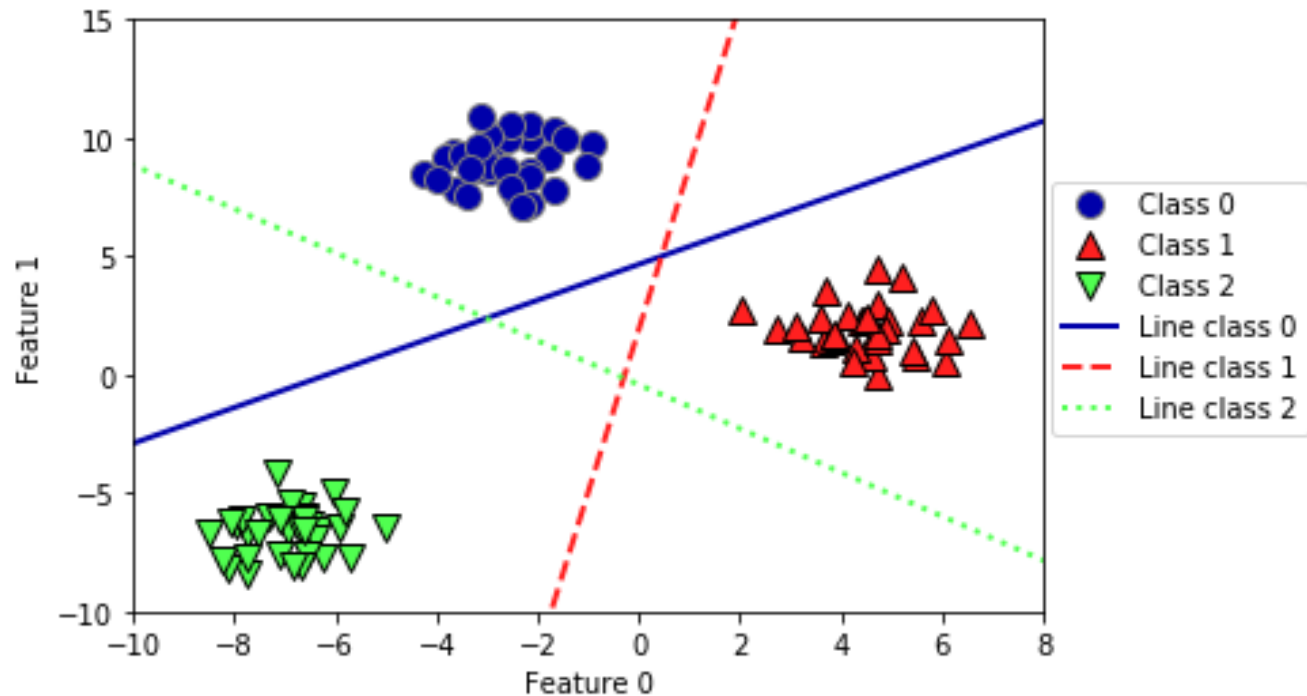
$$\begin{bmatrix} x_{1,0} & x_{1,1} & x_{1,2} & \cdots & x_{1,m} \\ x_{2,0} & x_{2,1} & x_{2,2} & \cdots & x_{2,m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{N,0} & x_{N,1} & x_{N,2} & \cdots & x_{N,m} \end{bmatrix} \begin{bmatrix} w_{0,1} & w_{0,2} & \cdots & w_{0,n} \\ w_{1,1} & w_{1,2} & \cdots & w_{1,n} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,1} & w_{m,2} & \cdots & w_{m,n} \end{bmatrix} = \begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,n} \\ y_{2,1} & y_{2,2} & \cdots & y_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ y_{N,1} & y_{N,2} & \cdots & y_{N,n} \end{bmatrix}$$

- Train one classifier for each class
 - (cf. Marsland's ch.3)
- Works for **multi-label classification**
- But the multi-class classifiers should only propose one class
- How to choose?



One vs. rest contd.

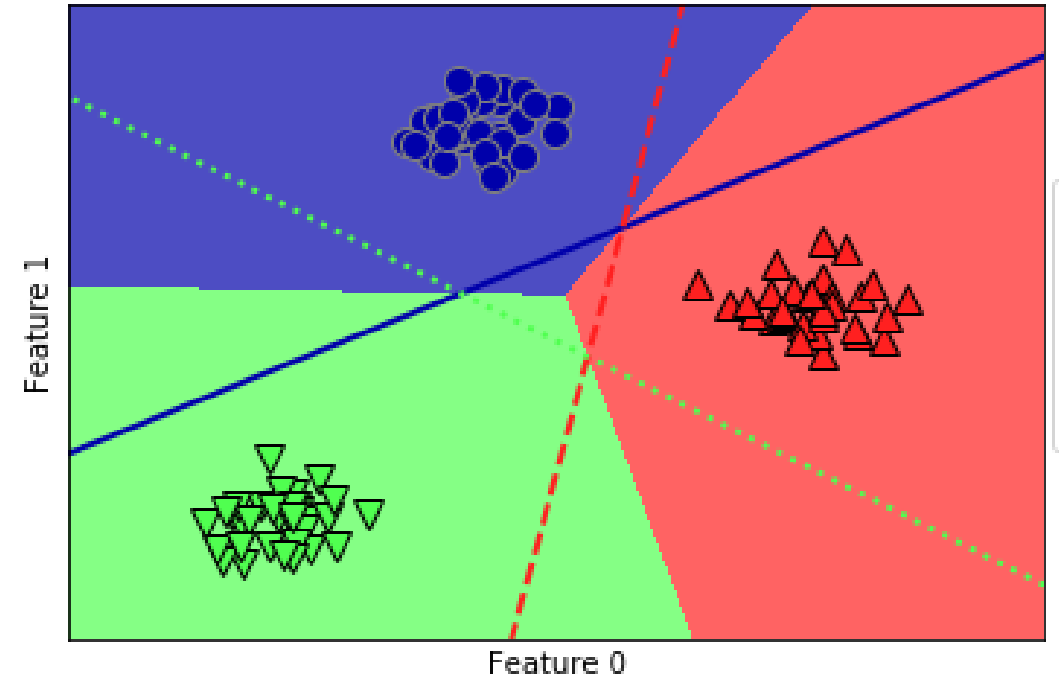
- It is easy to decide for items which fall into exactly one class
- But what if they fall into
 - More than one class?
 - No classes?



[https://github.com/amueller/introduction to ml with python](https://github.com/amueller/introduction%20to%20ml%20with%20python)

One vs. rest

- If each classifier predicts a score, compare the scores for the classes
- Choose the class with the highest score.
- E.g., log. reg.:
 - Probability of being **red**: 0.8
 - Probability of being **blue**: 0.7
 - Choose **red**



[https://github.com/amueller/introduction to ml with python](https://github.com/amueller/introduction%20to%20ml%20with%20python)

One vs. rest

$$\begin{bmatrix} x_{1,0} & x_{1,1} & x_{1,2} & \cdots & x_{1,m} \\ x_{2,0} & x_{2,1} & x_{2,2} & \cdots & x_{2,m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{N,0} & x_{N,1} & x_{N,2} & \cdots & x_{N,m} \end{bmatrix} \begin{bmatrix} w_{0,1} & w_{0,2} & \cdots & w_{0,n} \\ w_{1,1} & w_{1,2} & \cdots & w_{1,n} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,1} & w_{m,2} & \cdots & w_{m,n} \end{bmatrix} = \begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,n} \\ y_{2,1} & y_{2,2} & \cdots & y_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ y_{N,1} & y_{N,2} & \cdots & y_{N,n} \end{bmatrix}$$

- For x_i choose the j for which $y_{i,j}$ is the max of $\{y_{i,1}, y_{i,2}, \dots, y_{i,n}\}$

Multinomial Logistic Regression

- Logistic regression gives another option for making a multi-class classifier
- Called **multinomial logistic regression**, or **softmax regression**
 - also called **maximum entropy (maxent) classifier**,
- With one class we considered $P(t = 1|\vec{x}) = \frac{e^{\vec{w}\cdot\vec{x}}}{1+e^{\vec{w}\cdot\vec{x}}} = \frac{1}{1+e^{-\vec{w}\cdot\vec{x}}}$
- and implicitly $P(t = 0|\vec{x}) = 1 - \frac{e^{\vec{w}\cdot\vec{x}}}{1+e^{\vec{w}\cdot\vec{x}}} = \frac{1}{1+e^{\vec{w}\cdot\vec{x}}}$
- We now consider a linear expression \vec{w}_i , for **each class** $C_i, i = 1, \dots, k$
- The probability for each class is then given by the **softmax** function

$$P(C_j|\vec{x}) = \frac{e^{\vec{w}_j\cdot\vec{x}}}{\sum_{i=1}^k e^{\vec{w}_i\cdot\vec{x}}}$$

Training softmax

- It is possible to train towards softmax.
- In each step, we have to calculate y_j for each class j .
- In updating the weights for one class i , the predicted values for all the classes are considered and contribute to the update.
- We skip the details.