

Linear models II

Classification

How can we...

model nonlinear relationships using linear models?

use linear models for classification?

choose the parameters to fit a linear classification model to training data?

Can we model nonlinear relationships?

Linear models are linear in the **parameters**

A linear combination is quantity where a set of terms are added together, each multiplied by a constant (parameter) and adding the results

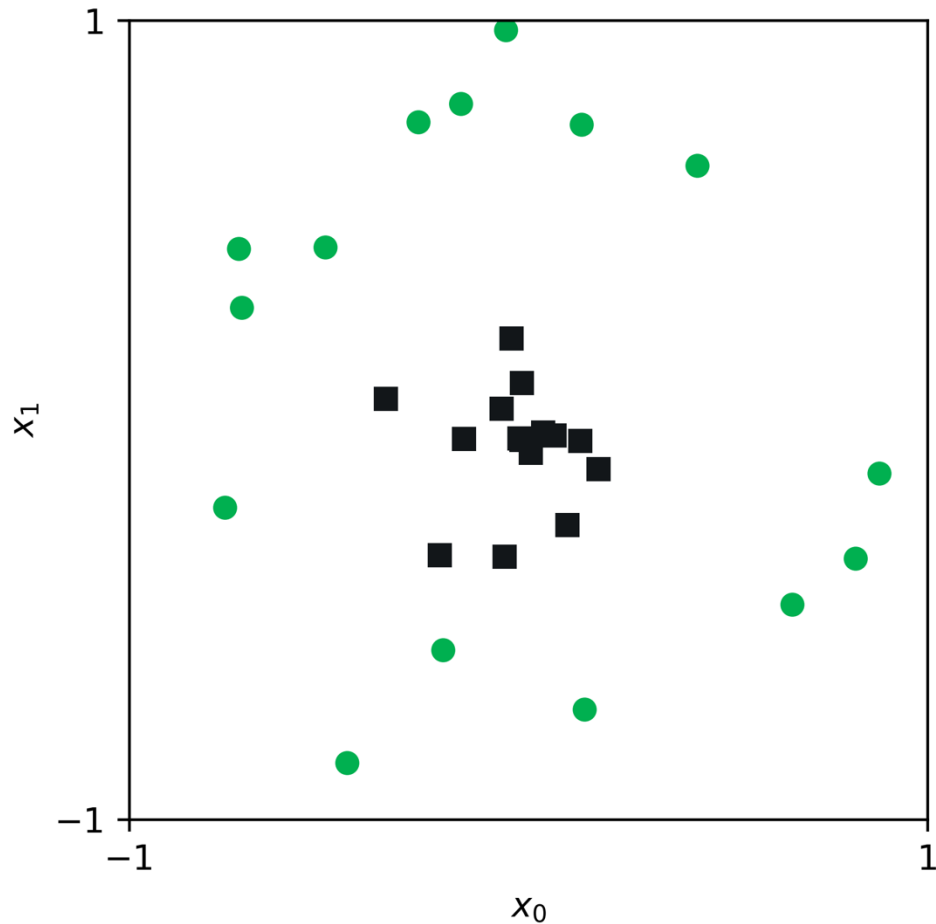
They can model **nonlinear relationships** between features and targets through **feature transformations**

There would need to be a linear relationship between the **transformed features** and the target variables for this to be effective

Limitations of linear decision boundaries

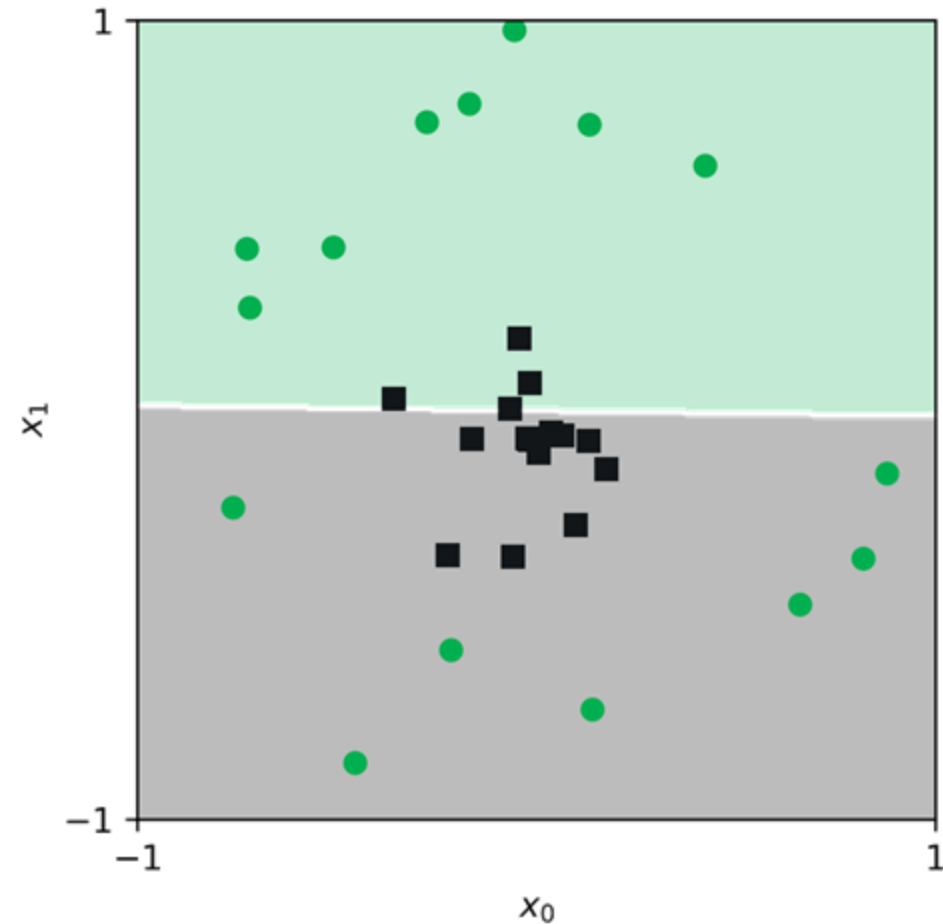
Original data

\mathbf{x}



Classify the features in this X -space

$$\hat{f}_x(\mathbf{x}) = \begin{cases} 1 & \mathbf{w}^T \mathbf{x} > 0 \\ 0 & \text{else} \end{cases}$$



Transformations of features

Consider a digits example...

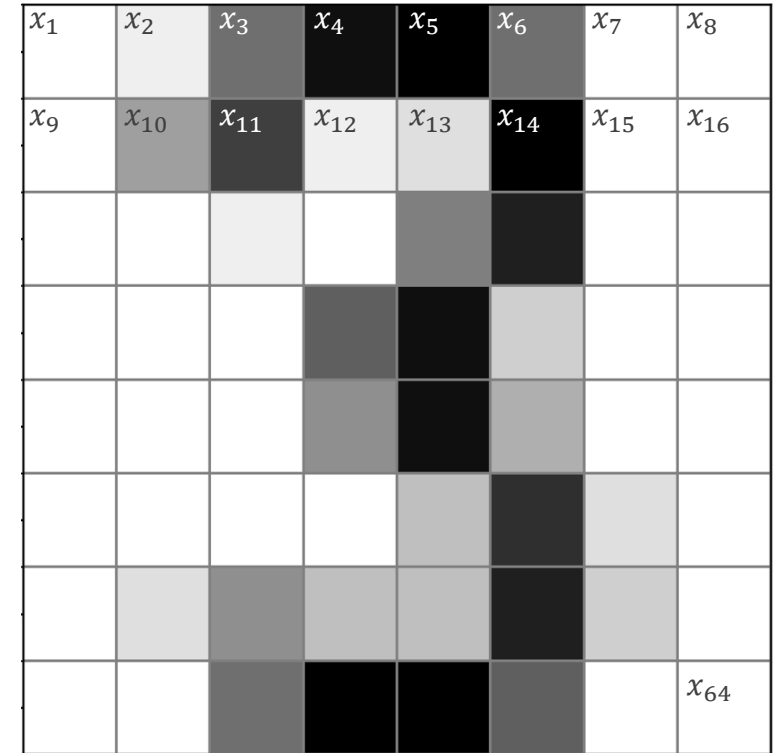
$$\mathbf{x} = [x_1, x_2, x_3, \dots, x_{64}]$$

We could **design features** based on the original features. For example:

$$\mathbf{z} = [x_5 x_{11}, x_{14}^2, \frac{x_{64}}{x_{14}}]$$

Which can be written simply as
variables in a new feature space:

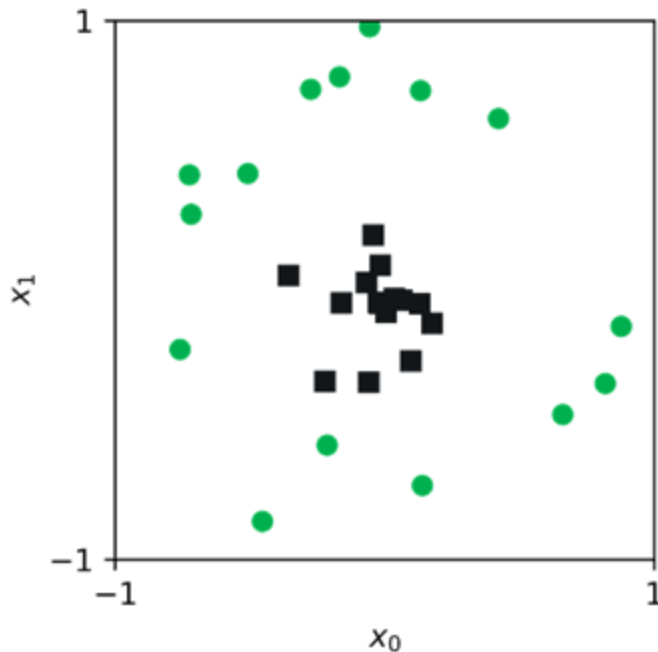
$$\mathbf{z} = [z_1, z_2, z_3]$$



Source: Abu-Mostafa, Learning from Data, Caltech

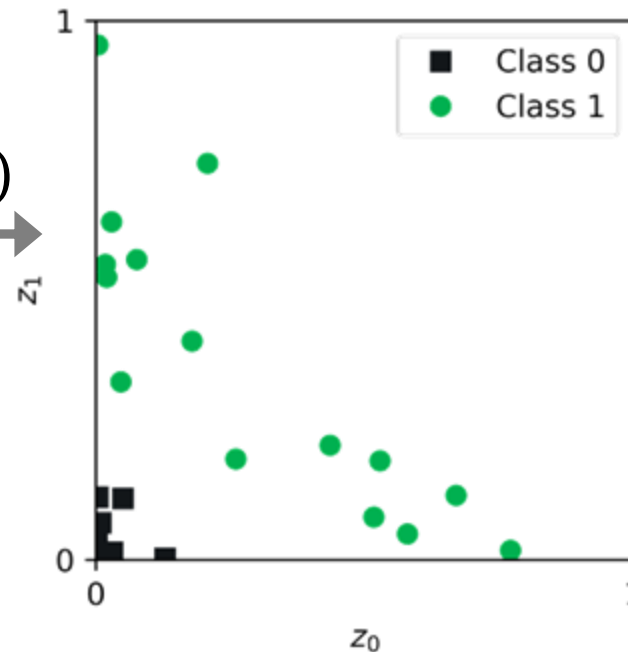
1

Original data
 \mathbf{x}



transform
the data

$$\mathbf{z} = \Phi(\mathbf{x})$$



2

This example transform is
quadratic

$$z_i = \Phi(x_i) = x_i^2$$

$$z_0 = x_0^2$$

$$z_1 = x_1^2$$

Classify the features
in this Z-space

$$\hat{f}_z(\mathbf{z}) = \begin{cases} 1 & \mathbf{w}^T \mathbf{z} > 0 \\ 0 & \text{else} \end{cases}$$

A new
representation
of our data

3

Predictions in the
original X-space

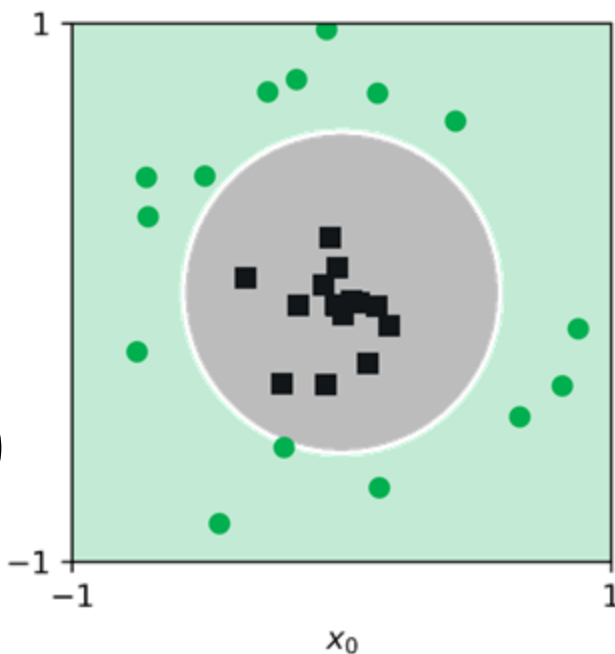
$$\hat{f}(\mathbf{x}) = \hat{f}_z(\Phi(\mathbf{x}))$$

$$\mathbf{x} = \Phi^{-1}(\mathbf{z})$$

transform
the data back

$$x_0 = z_0^{1/2}$$

$$x_1 = z_1^{1/2}$$

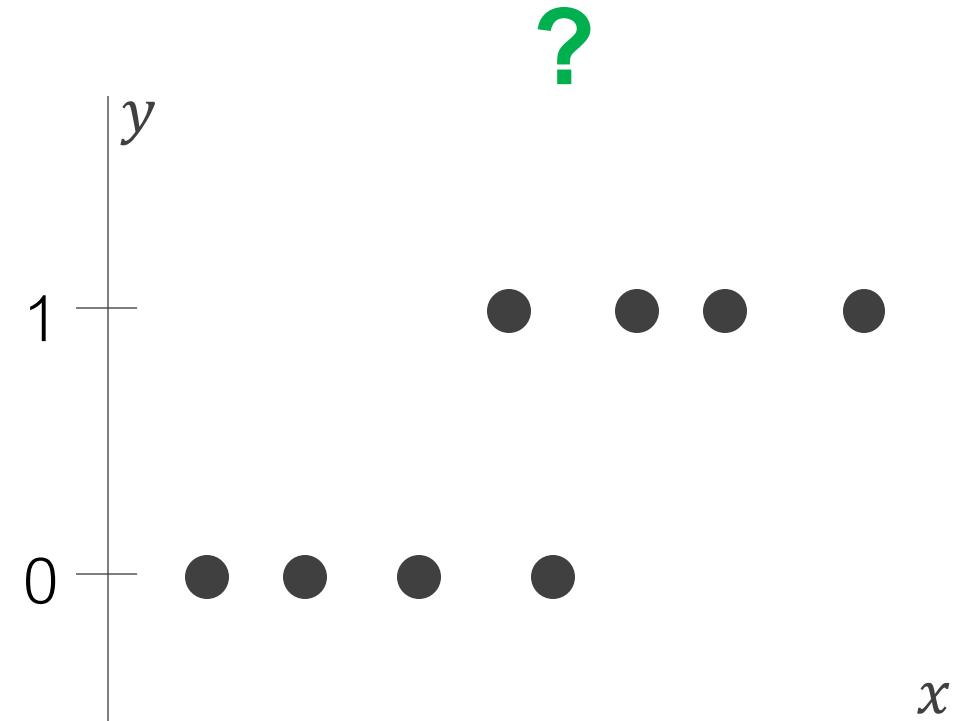
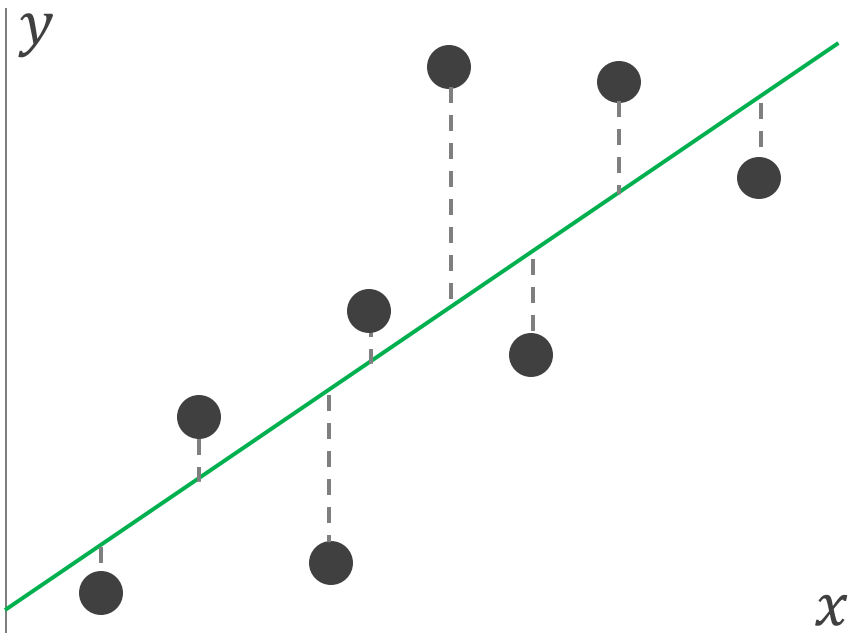


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So how do we use linear models for classification?

How do we fit linear models for classification?

Linear regression



Moving from regression to classification

Regression

$$y = \sum_{i=0}^p w_i x_i$$

Classification
(perceptron)

$$y = \text{sign} \left(\sum_{i=0}^p w_i x_i \right)$$

$$y = \begin{cases} 1 & \sum_{i=0}^p w_i x_i > 0 \\ -1 & \text{else} \end{cases}$$

where

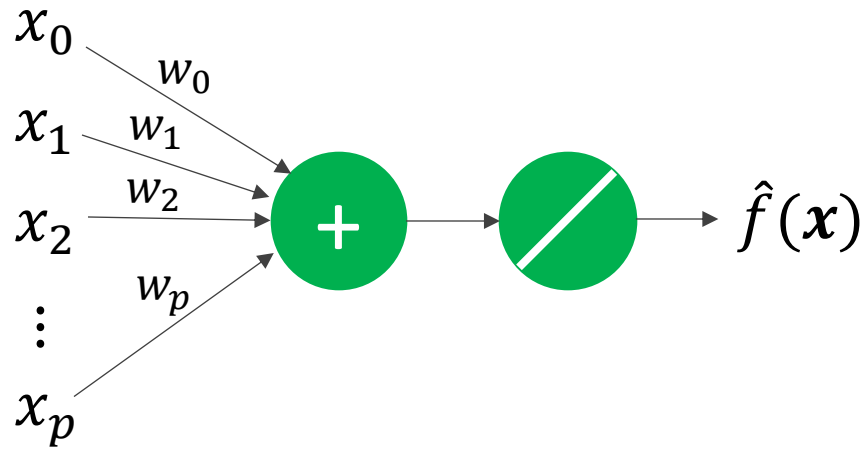
$$\text{sign}(x) = \begin{cases} 1 & x > 0 \\ -1 & \text{else} \end{cases}$$

Source: Abu-Mostafa, Learning from Data, Caltech

Moving from regression to classification

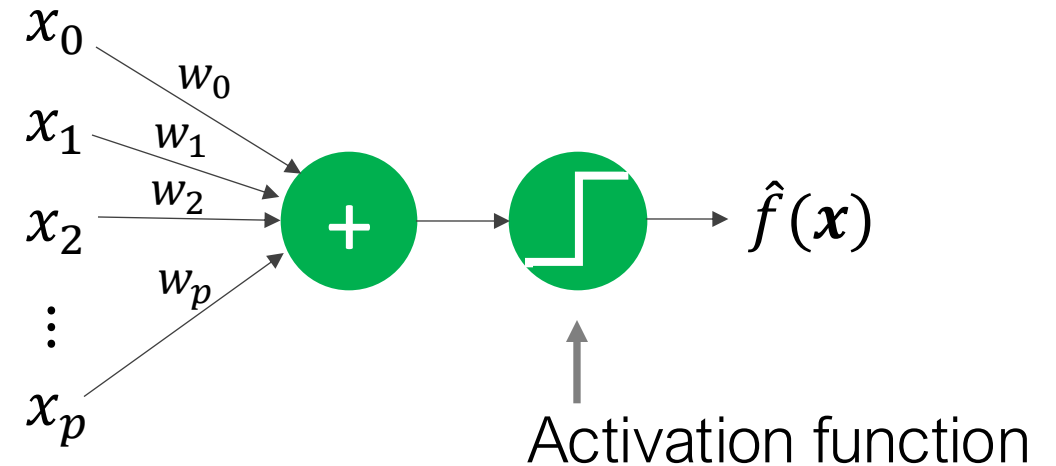
Linear Regression

$$\hat{f}(\mathbf{x}) = \sum_{i=0}^p w_i x_i$$



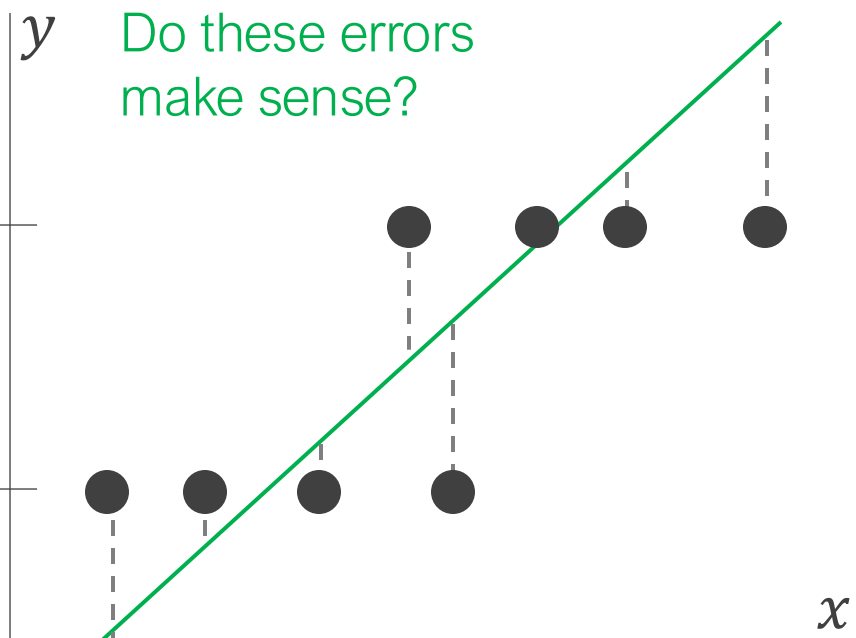
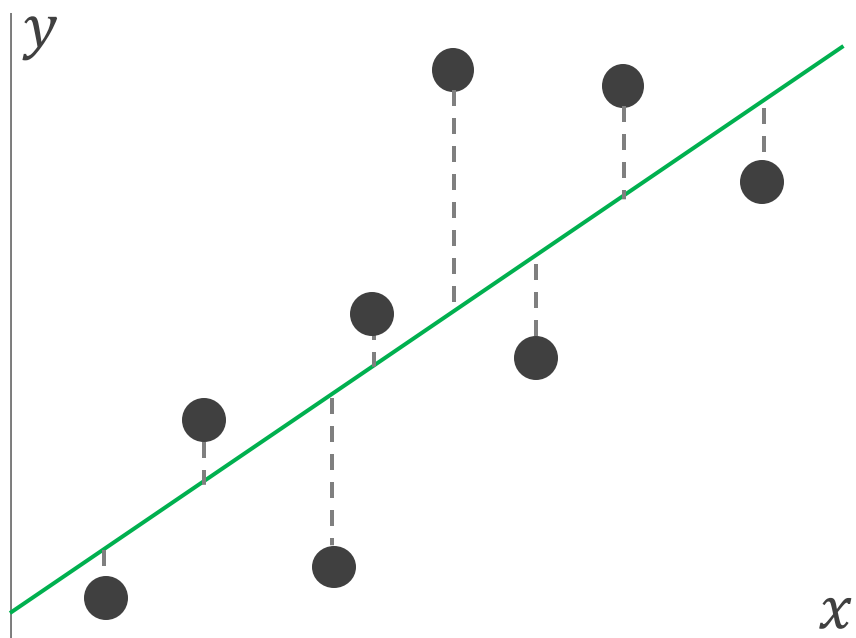
Linear Classification (perceptron)

$$\hat{f}(\mathbf{x}) = \text{sign} \left(\sum_{i=0}^p w_i x_i \right)$$



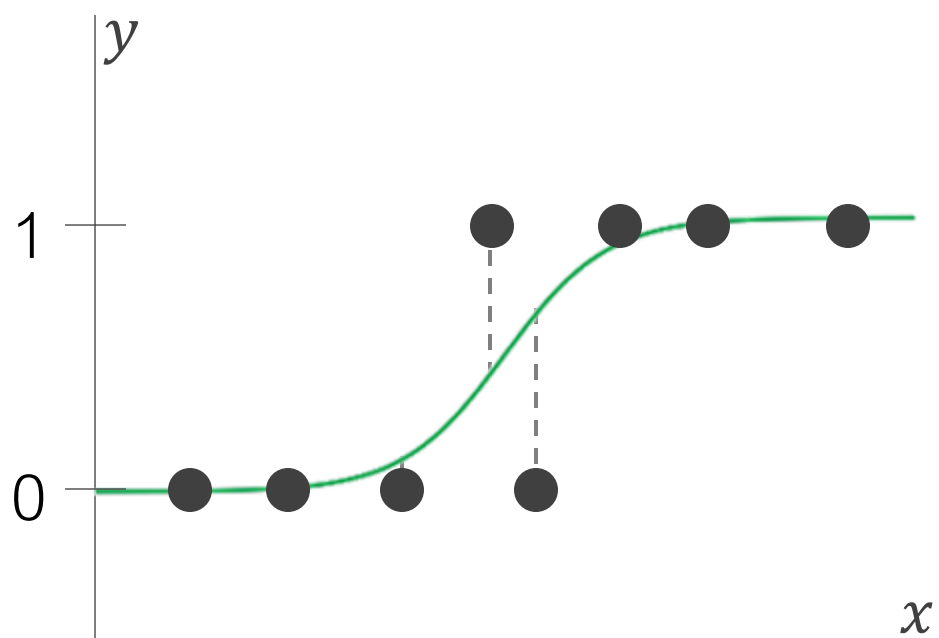
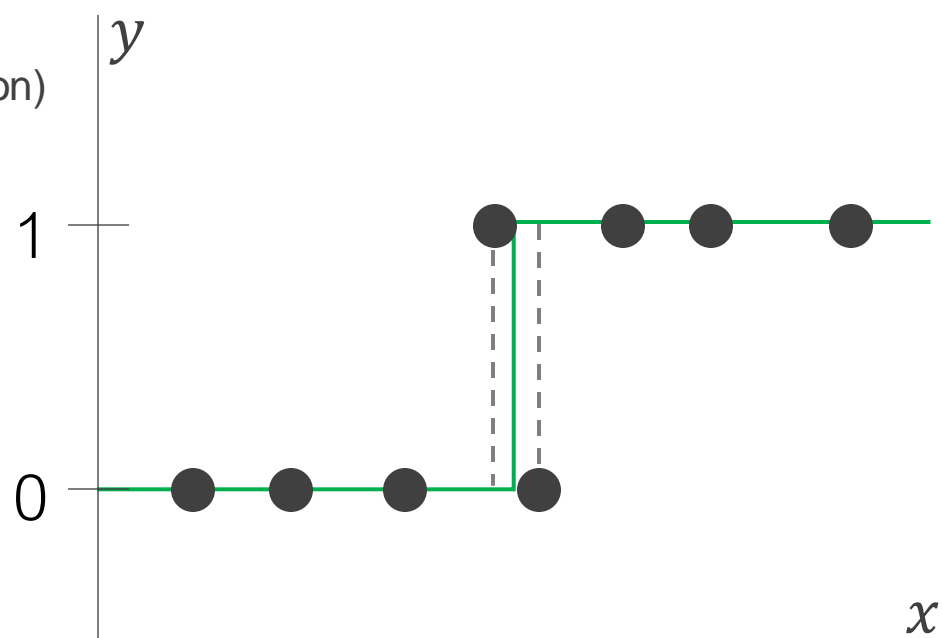
Source: Abu-Mostafa, Learning from Data, Caltech

Linear regression
(linear activation)



Linear regression
applied to a
classification
problem
(linear activation)

Perceptron
(sign activation)



Logistic regression
(sigmoid activation)

Sigmoid function

Definition

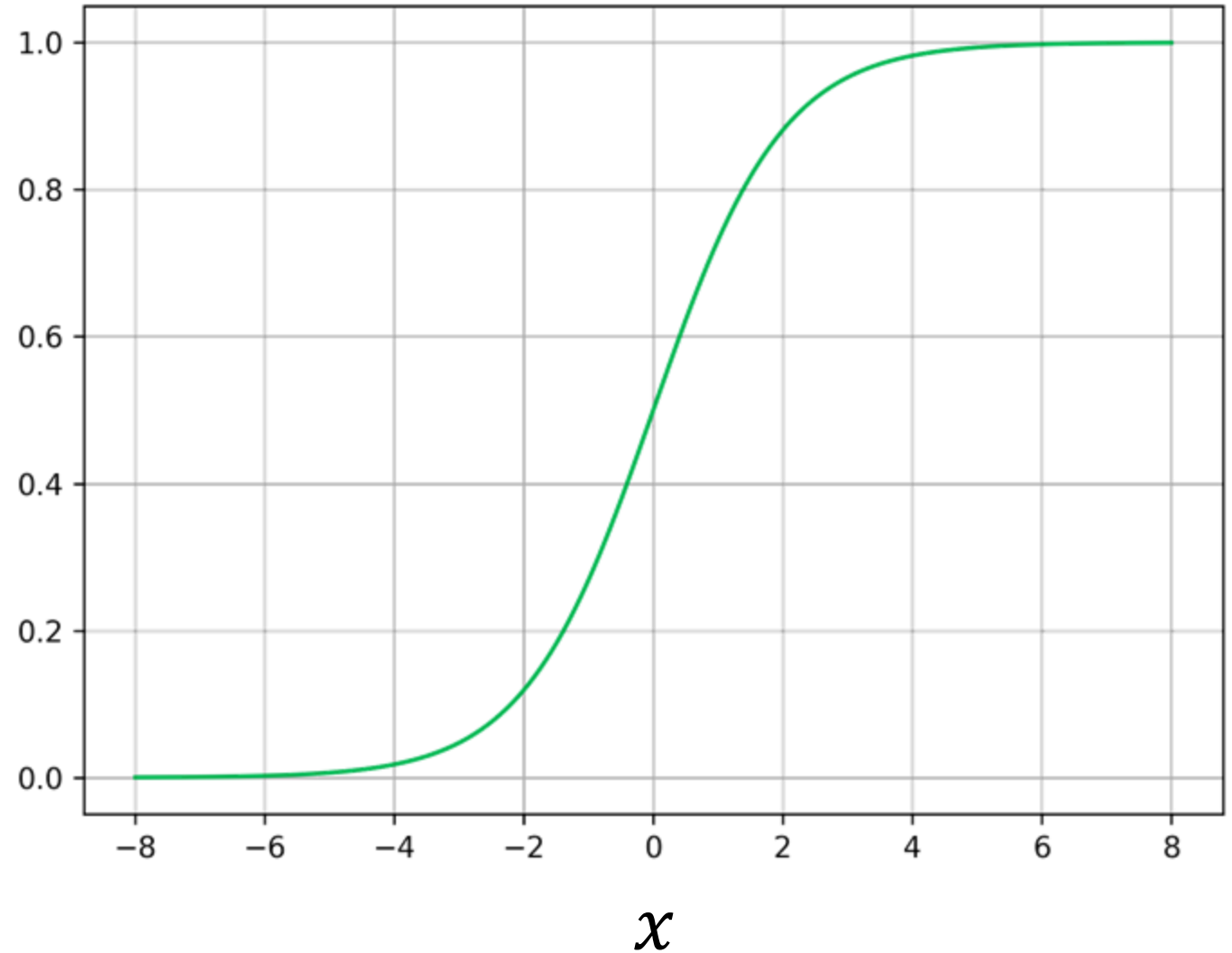
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

σ

Useful properties

$$\sigma(-x) = 1 - \sigma(x)$$

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1 - \sigma(x))$$



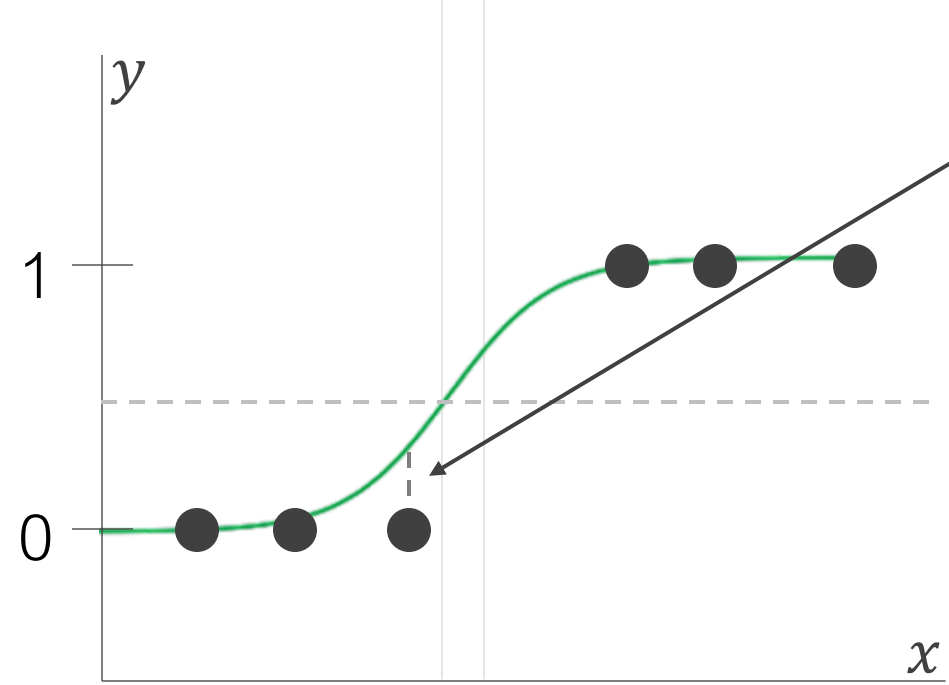
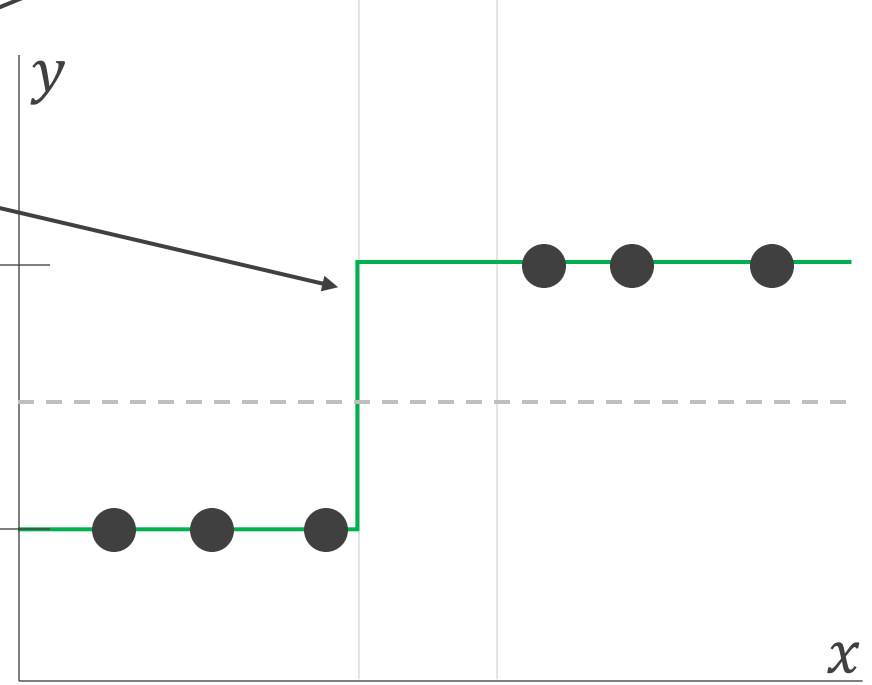
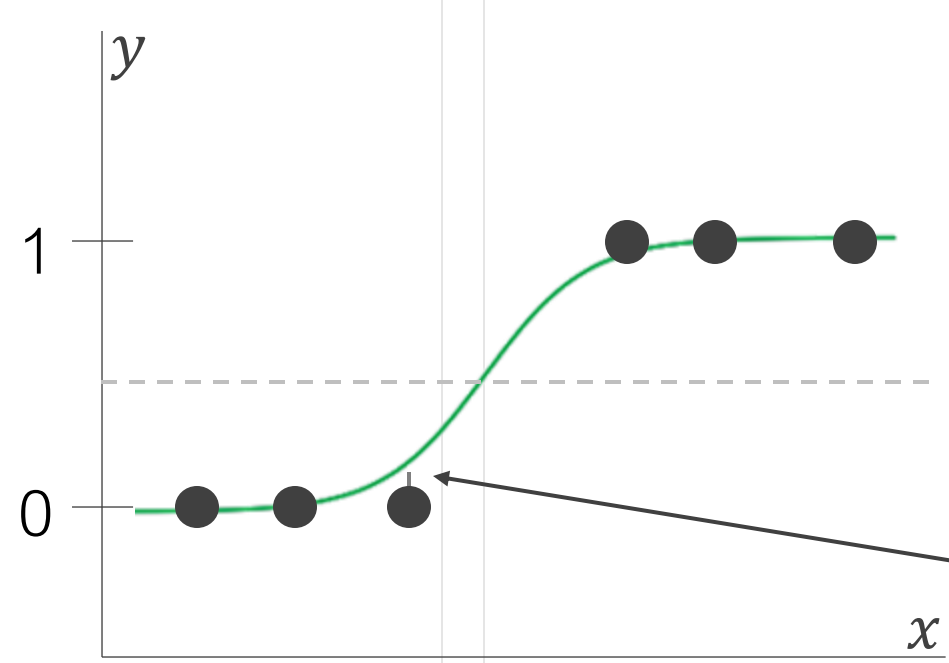
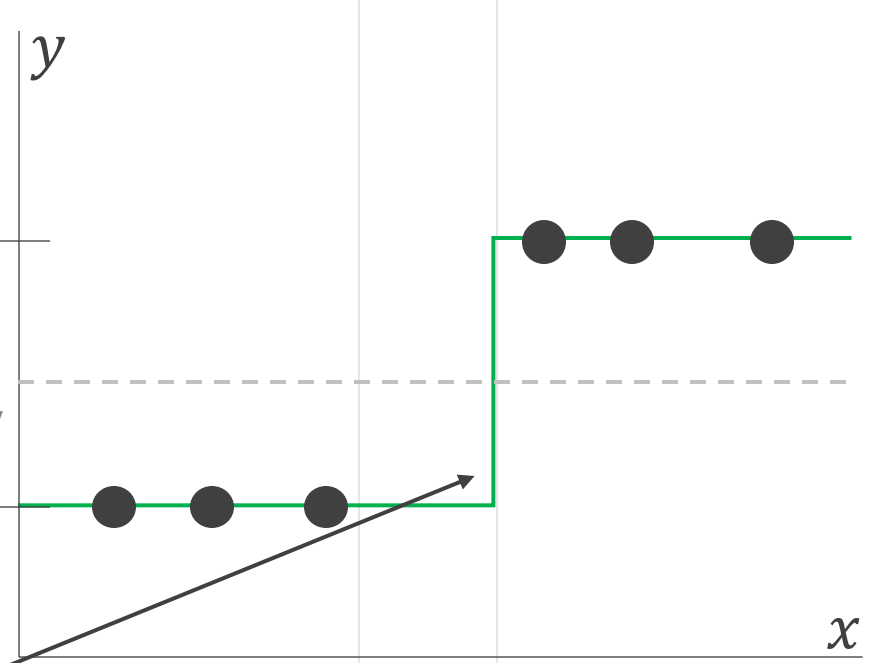
Perceptron (sign activation)

Logistic regression (sigmoid activation)

Both
decision
boundaries
incur the
same loss

The sigmoid
assigns error
to samples
close to the
margin

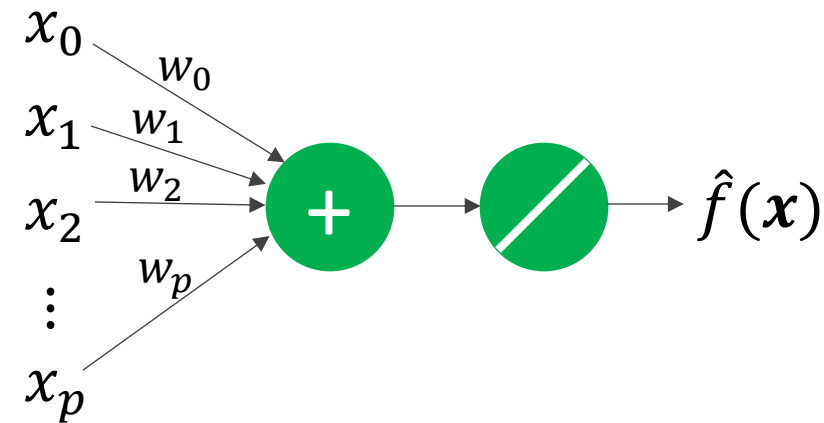
Favors a
larger margin



Moving from regression to classification

Linear Regression

$$\hat{f}(\mathbf{x}) = \sum_{i=0}^p w_i x_i$$

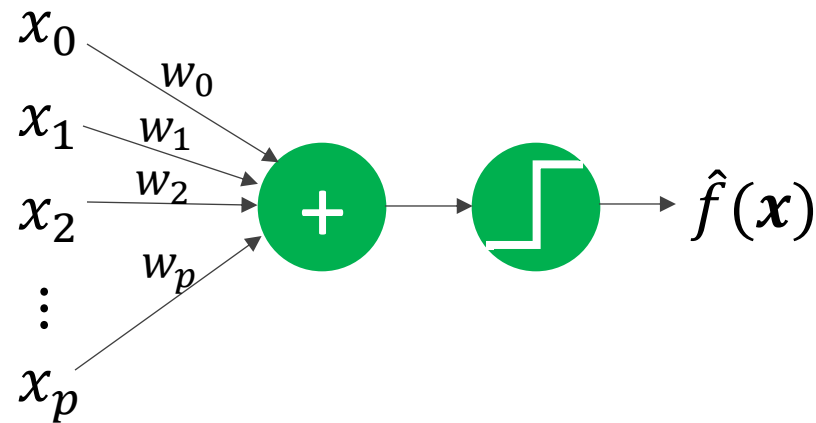


Linear Classification

Perceptron

$$\hat{f}(\mathbf{x}) = \text{sign} \left(\sum_{i=0}^p w_i x_i \right)$$

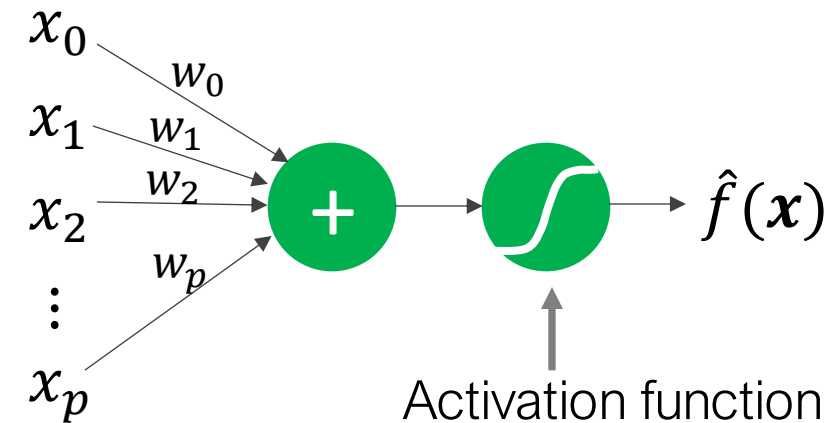
$$\text{sign}(x) = \begin{cases} 1 & x > 0 \\ -1 & \text{else} \end{cases}$$



Logistic Regression

$$\hat{f}(\mathbf{x}) = \sigma \left(\sum_{i=0}^p w_i x_i \right)$$

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



Source: Abu-Mostafa, Learning from Data, Caltech

We fit our model to training data

1. Choose a **hypothesis set of models** to train
2. Identify a **cost function** to measure the model fit to the training data
3. **Optimize** model **parameters** to minimize cost

For linear regression the steps were (i.e. OLS):

- a. Calculate the gradient of the cost function
- b. Set the gradient to zero
- c. Solve for the model parameters

When this approach is not an option, we often use **gradient descent**

For classification we COULD try the same cost function as regression

Assume the cost function is **mean square error**

$$C(\mathbf{w}) \triangleq E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (\hat{f}(\mathbf{x}_n, \mathbf{w}) - y_n)^2$$

Plug in our model

$$C(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (\sigma(\mathbf{w}^T \mathbf{x}_n) - y_n)^2$$

$$\hat{f}(\mathbf{x}_n, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x}_n)$$

Calculate the gradient

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \frac{2}{N} \sum_{n=1}^N [\sigma(\mathbf{w}^T \mathbf{x}_n) - y_n] \sigma(\mathbf{w}^T \mathbf{x}_n) [1 - \sigma(\mathbf{w}^T \mathbf{x}_n)] \mathbf{x}_n$$

Set the gradient to zero and minimize to solve for \mathbf{w}

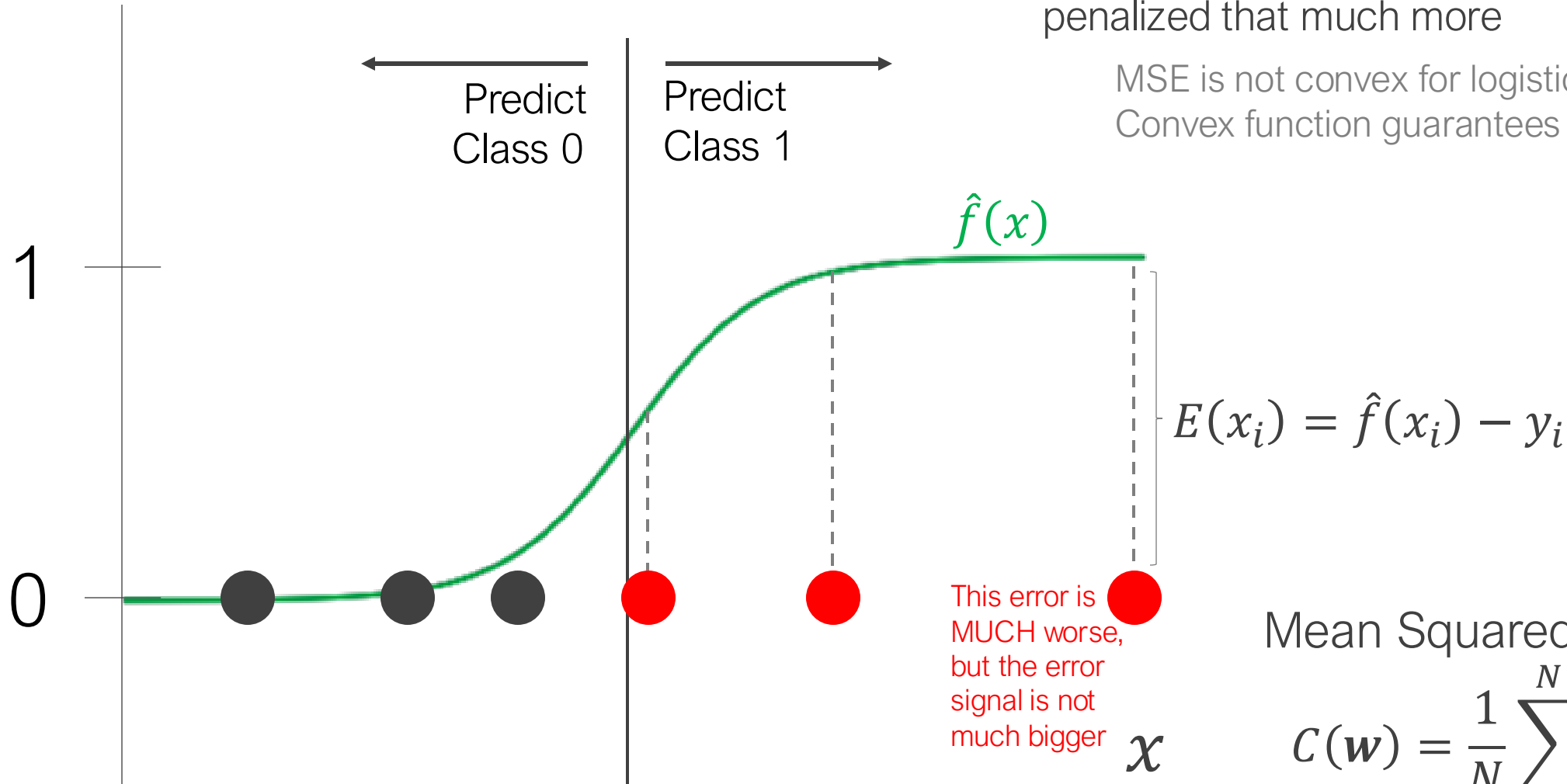
$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \mathbf{0}$$

But does MSE make sense for classification?

MSE for classification

Intuition: With a mean squared error cost function, bigger classification mistakes are not penalized that much more

MSE is not convex for logistic regression
Convex function guarantees a global minimum



Mean Squared Error Cost:

$$C(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (\hat{f}(\mathbf{x}_n, \mathbf{w}) - y_n)^2$$

We need a different cost function for logistic regression...

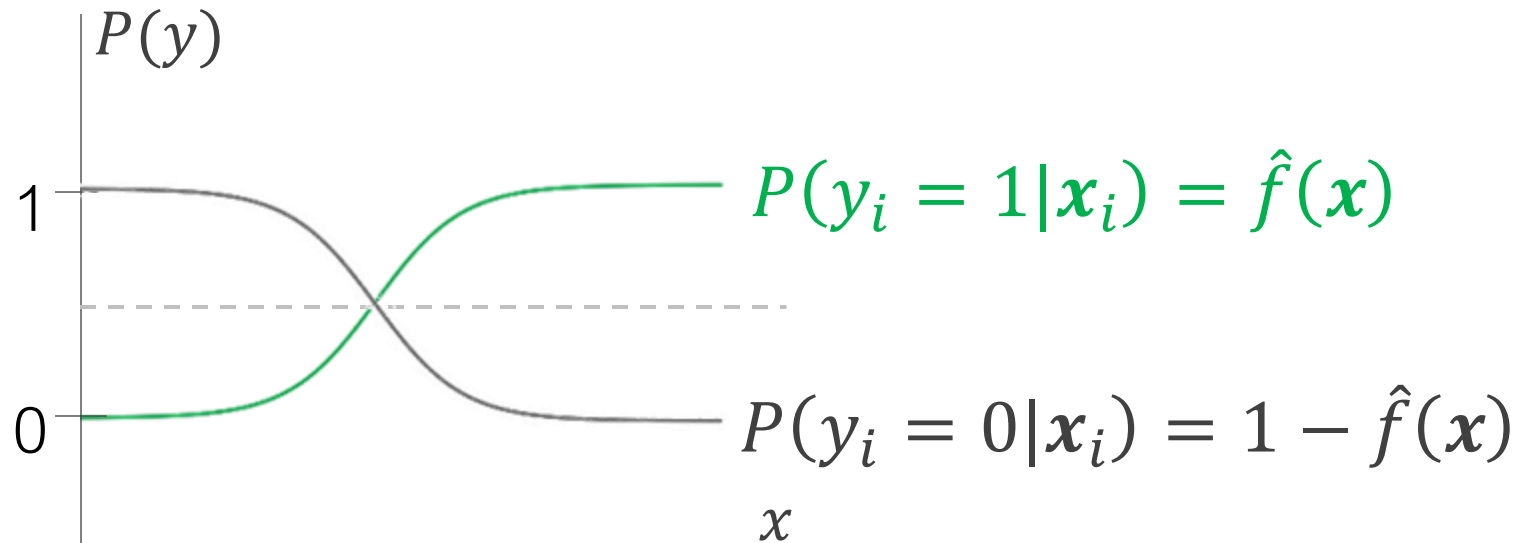
Is there a better cost function we could use for classification problems...?

Another interpretation of logistic regression

Our model: $\hat{y} = \hat{f}(\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x})$

$$\sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

Logistic regression models the
conditional probability that a sample belongs to a class



What's linear about logistic regression?

$$\hat{f}(\mathbf{x}) = \hat{y} = \sigma(\mathbf{w}^T \mathbf{x})$$

$$\hat{y} = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

$$\frac{1}{\hat{y}} = 1 + e^{-\mathbf{w}^T \mathbf{x}}$$

$$\frac{1}{\hat{y}} - 1 = e^{-\mathbf{w}^T \mathbf{x}}$$

$$\frac{1}{\hat{y}} - \frac{\hat{y}}{\hat{y}} = e^{-\mathbf{w}^T \mathbf{x}}$$

$$\frac{1 - \hat{y}}{\hat{y}} = e^{-\mathbf{w}^T \mathbf{x}}$$

$$\frac{1 - \hat{y}}{\hat{y}} = e^{-\mathbf{w}^T \mathbf{x}}$$

$$\log\left(\frac{1 - \hat{y}}{\hat{y}}\right) = \log(e^{-\mathbf{w}^T \mathbf{x}})$$

$$\log\left(\frac{1 - \hat{y}}{\hat{y}}\right) = -\mathbf{w}^T \mathbf{x}$$

$$-\log\left(\frac{1 - \hat{y}}{\hat{y}}\right) = \mathbf{w}^T \mathbf{x}$$

$$\log\left(\frac{\hat{y}}{1 - \hat{y}}\right) = \mathbf{w}^T \mathbf{x}$$

If we interpret our target variable, \hat{y} , as the probability of class 1, then $\mathbf{w}^T \mathbf{x}$ models the log odds ratio

$$\hat{y} = P(Y = 1 | \mathbf{x})$$

$$\log\left[\frac{P(Y = 1 | \mathbf{x})}{1 - P(Y = 1 | \mathbf{x})}\right] = \mathbf{w}^T \mathbf{x}$$

$$\log\left[\frac{P(Y = 1 | \mathbf{x})}{P(Y = 0 | \mathbf{x})}\right] = \mathbf{w}^T \mathbf{x}$$

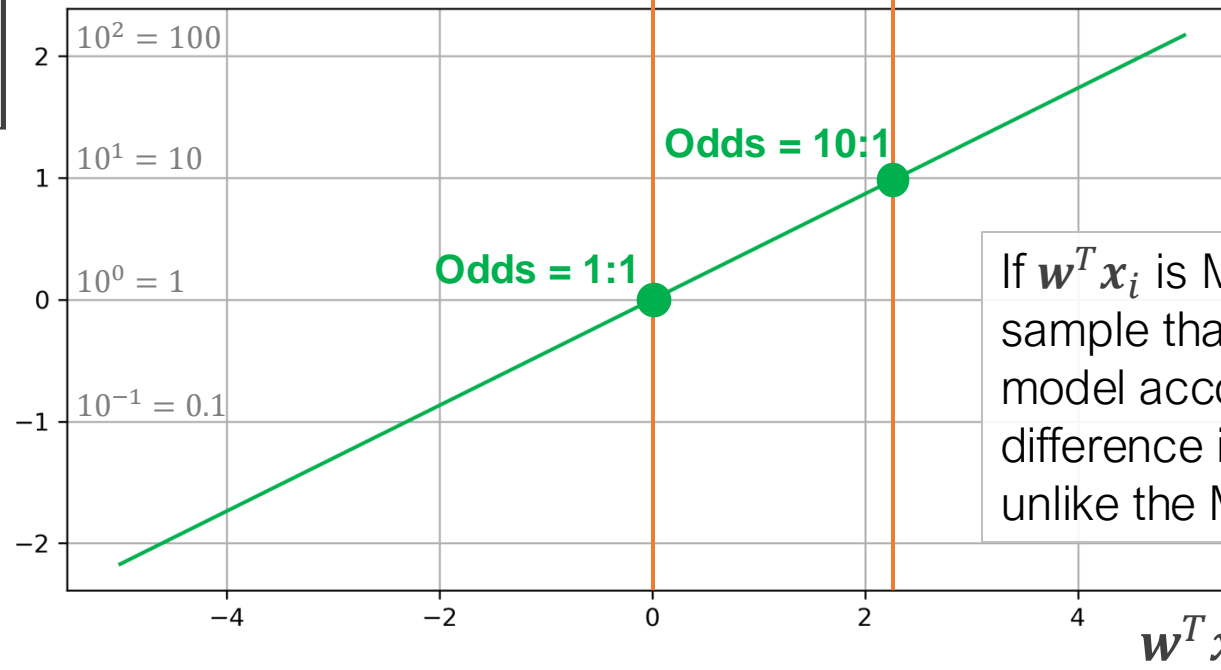
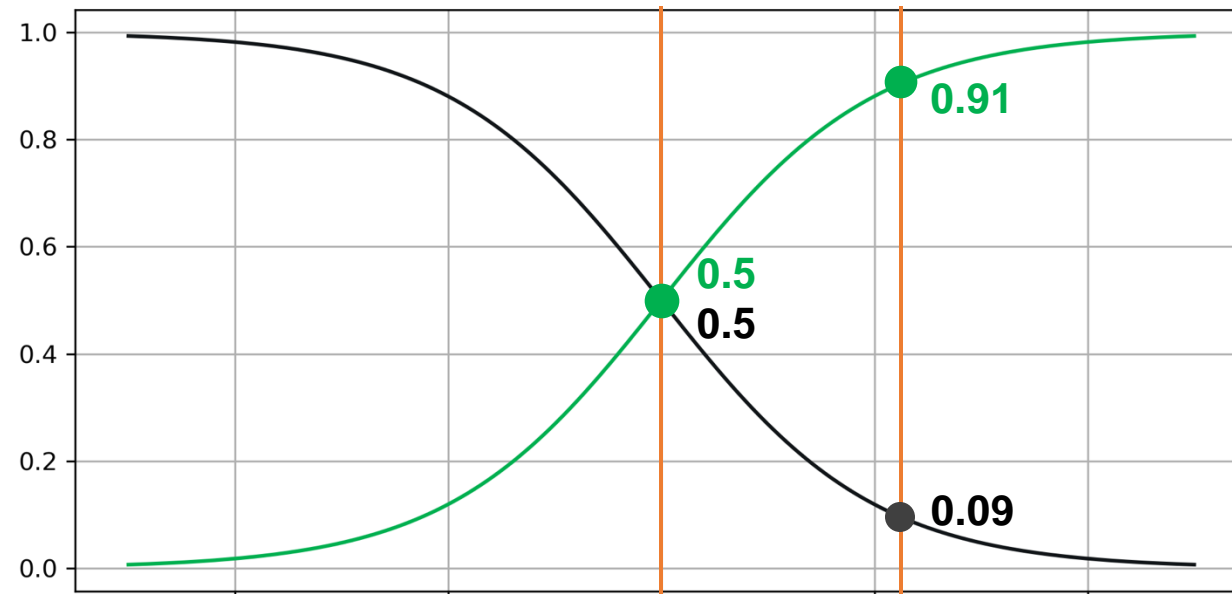
Interpretation of the odds ratio

Log-odds ratio:
ratio of positive class
probability to the
negative class

$$\log \left[\frac{P(y_i = 1 | \mathbf{x}_i)}{P(y_i = 0 | \mathbf{x}_i)} \right]$$

The log-odds ratio is a linear
function of the features

$$P(y_i | \mathbf{x}_i)$$



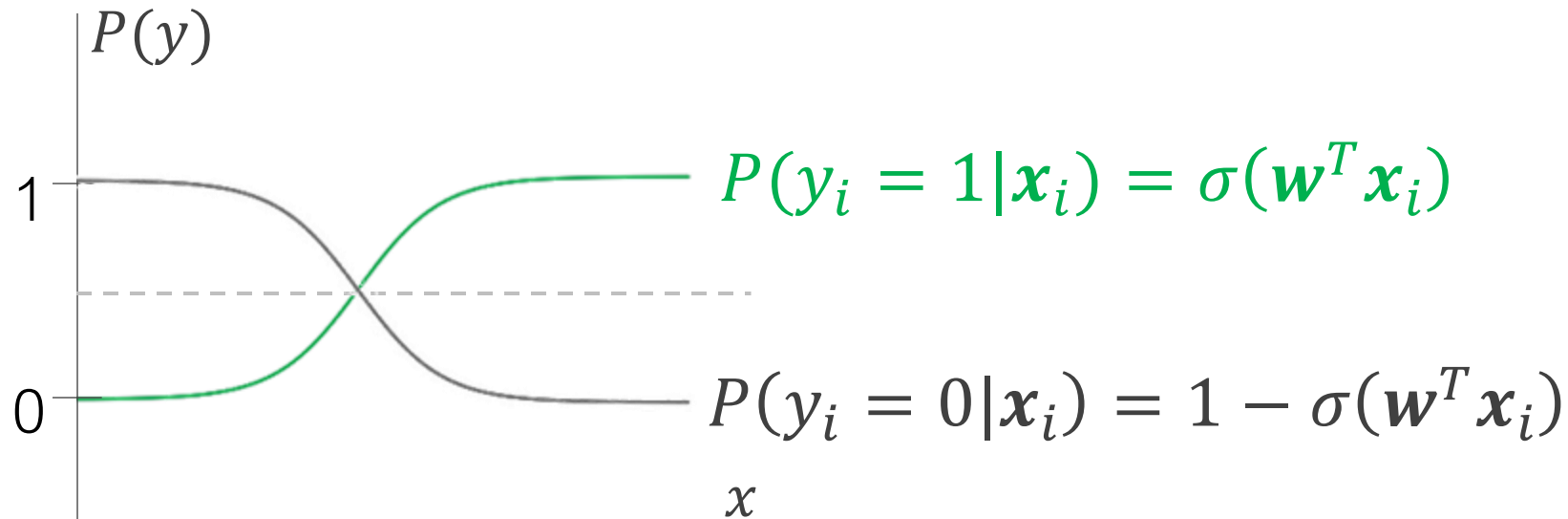
If $\mathbf{w}^T \mathbf{x}_i$ is MUCH larger for one sample than another, this model accounts for this difference in the odds ratio unlike the MSE approach

So how do we fit our model to the data in this case?

Our model: $\hat{y} = \hat{f}(\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x})$

$$\sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

Logistic regression models the
conditional probability that a sample belongs to a class



Sidebar: Maximum Likelihood Estimation



We want to determine the underlying probability of the coin landing on “heads”; the coin could be biased.

We flip the coin 1,000 times

...in other words, we have $N = 1,000$ **independent** Bernoulli trials

Coin flips, binary outcomes

$$P(X = 1) = p$$

$$P(X = 0) = 1 - p$$

Goal: find the value of p that maximizes the likelihood function

Interpretation of likelihood: a function of a parameter we want optimize for, given our data: $L(p|x)$

Goal: find the value of p that maximizes the likelihood of our data

$$P(X = 1) = p$$

$$P(X = 0) = 1 - p$$

For a **single observation**, the likelihood is:

$$L(p|x_i) = P(x_i|p) = p^{x_i}(1 - p)^{1-x_i}$$

For **multiple independent observations**, the likelihood is:

For independent random events, the probability of both events is the product of their individual probabilities:

$$P(A \text{ and } B) = P(A)P(B)$$

$$L(p|\mathbf{x}) = P(\mathbf{x}|p) = \prod_{i=1}^N P(x_i|p)$$

$$= p^{\sum_{i=1}^N x_i} (1 - p)^{N - \sum_{i=1}^N x_i}$$

Goal: find the value of p that maximizes the likelihood of our data

$$L(p) = p^{\sum x_i} (1 - p)^{N - \sum x_i}$$

Here, $L(p)$ is short for $L(p|\mathbf{x})$

Maximizing the likelihood is equivalent to maximizing the log-likelihood

$$\ln[L(p)] = \ln[p^{\sum x_i} (1 - p)^{N - \sum x_i}]$$

$$\ln[L(p)] = \ln(p) \sum_{i=1}^N x_i + \ln(1 - p) \left[N - \sum_{i=1}^N x_i \right]$$

To **maximize the likelihood**, we take the **derivative of this log likelihood** and **set it to zero**, then solve for p

Goal: find the value of p that maximizes the likelihood of our data

We take the derivative of this log likelihood and set it to zero, then solve for p

$$\ln[L(p)] = \ln(p) \sum_{i=1}^N x_i + \ln(1-p) \left[N - \sum_{i=1}^N x_i \right]$$
$$\frac{\partial \ln[L(p)]}{\partial p} = \frac{\sum_{i=1}^N x_i}{p} - \frac{N - \sum_{i=1}^N x_i}{1-p} = 0$$

This results in our estimate being the mean of our observations:

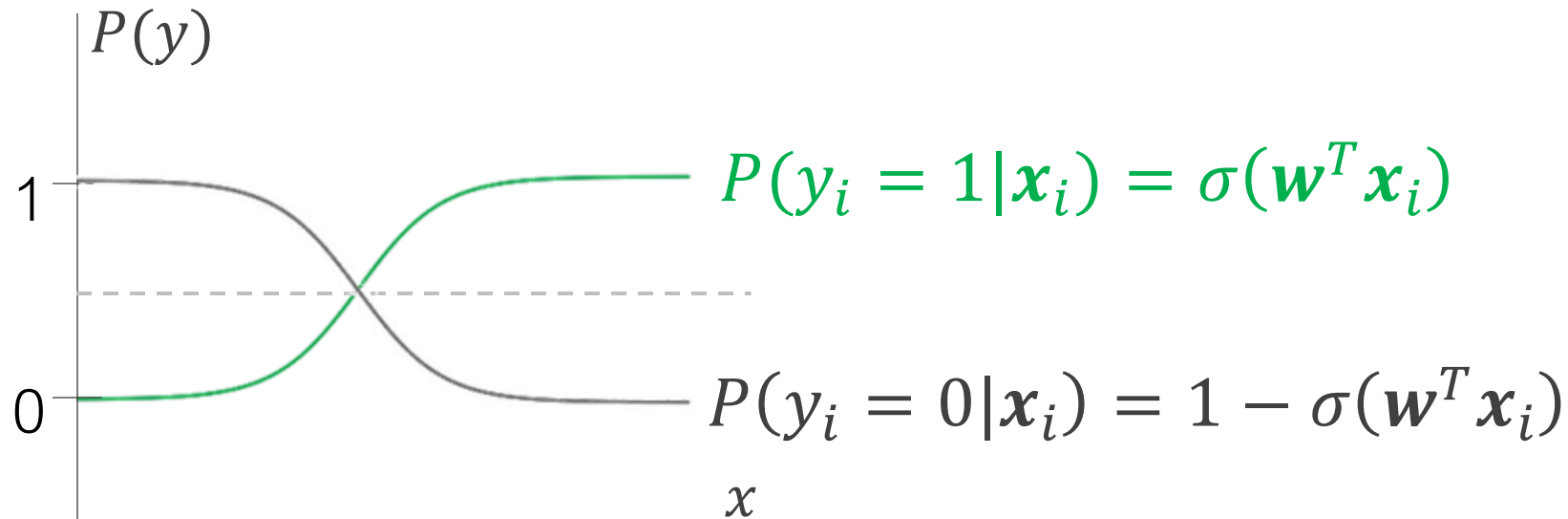
$$\hat{p} = \frac{1}{N} \sum_{i=1}^N x_i$$

Applying this to logistic regression...

Our model: $\hat{y} = \hat{f}(\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x})$

$$\sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

Logistic regression models the
conditional probability that a sample belongs to a class



Note these are
both functions of
our parameters, \mathbf{w}

The interpretation of the **Likelihood**

With class labels y_1, y_2, \dots, y_N and corresponding to $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$

The likelihood for **one observation**:

$$L(\mathbf{w}|y_i, \mathbf{x}_i) = P(y_i = 1|\mathbf{x}_i)^{y_i}P(y_i = 0|\mathbf{x}_i)^{1-y_i}$$

We're interested in the likelihood of the model as a function of the model parameters, \mathbf{w} . So $P(y_i|\mathbf{x}_i)$ is a function of \mathbf{w} .

$$L(\mathbf{w}) \triangleq P(\mathbf{y}|\mathbf{X})$$

The likelihood for **all observations**:

$$L(\mathbf{w}|\mathbf{y}, \mathbf{X}) = P(y_1, y_2, \dots, y_N|\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \prod_{i=1}^N P(y_i|\mathbf{x}_i)$$

Source: Malik Magdon-Ismail, Learning from Data

The likelihood for all observations:

$$L(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \prod_{i=1}^N P(y_i|\mathbf{x}_i) = \prod_{i=1}^N P(y_i = 1|\mathbf{x}_i)^{y_i} P(y_i = 0|\mathbf{x}_i)^{1-y_i}$$

Substituting:

$$P(y_i = 1|\mathbf{x}_i) = \sigma(\mathbf{w}^T \mathbf{x}_i)$$
$$P(y_i = 0|\mathbf{x}_i) = 1 - \sigma(\mathbf{w}^T \mathbf{x}_i)$$

$$= \prod_{i=1}^N \sigma(\mathbf{w}^T \mathbf{x}_i)^{y_i} [1 - \sigma(\mathbf{w}^T \mathbf{x}_i)]^{1-y_i}$$

We want to **MAXIMIZE the likelihood (minimize its negative)**

We can take the **logarithm**, negate it to get our **cost function**, then minimize it (using the gradient)

A little algebra

$$\begin{aligned} L(\mathbf{w}|\mathbf{y}, \mathbf{X}) &= \prod_{i=1}^N \sigma(\mathbf{w}^T \mathbf{x}_i)^{y_i} [1 - \sigma(\mathbf{w}^T \mathbf{x}_i)]^{1-y_i} \\ &= \prod_{i=1}^N \hat{y}_i^{y_i} [1 - \hat{y}_i]^{1-y_i} \quad \text{assuming} \quad \hat{y}_i \triangleq \sigma(\mathbf{w}^T \mathbf{x}_i) \end{aligned}$$

If we take the log of both sides:

$$\begin{aligned} \log L(\mathbf{w}|\mathbf{y}, \mathbf{X}) &= \log \left[\prod_{i=1}^N \hat{y}_i^{y_i} [1 - \hat{y}_i]^{1-y_i} \right] = \sum_{i=1}^N \log(\hat{y}_i^{y_i} [1 - \hat{y}_i]^{1-y_i}) \\ &= \sum_{i=1}^N y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i) \end{aligned}$$

Recall that
 $\log(ab) = \log(a) + \log(b)$
 $\log(a^b) = b \log(a)$

$$\log L(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \sum_{i=1}^N y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)$$

We can define our
cost function: $C(\mathbf{w}) = -\log L(\mathbf{w}|\mathbf{y}, \mathbf{X})$

$$C(\mathbf{w}) = - \left[\sum_{i=1}^N y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i) \right]$$

This quantity is often normalized by
dividing by N for interpreting the
results as **mean cost per sample**

For logistic regression,
 $\hat{y}_i \triangleq \sigma(\mathbf{w}^T \mathbf{x}_i)$

This is the cross entropy cost function

Cross Entropy

$$C(\mathbf{w}) = -\frac{1}{N} \left[\sum_{i=1}^N y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i) \right]$$

Per sample cost:

$$-y_i \log(\hat{y}_i) - (1 - y_i) \log(1 - \hat{y}_i)$$

When $y_i = 0$

$$\underbrace{-y_i}_{0} \log(\hat{y}_i) - \underbrace{(1 - y_i)}_1 \log(1 - \hat{y}_i)$$

The cost is:

$$-\log(1 - \hat{y}_i)$$

When $y_i = 1$

$$\underbrace{-y_i}_1 \log(\hat{y}_i) - \underbrace{(1 - y_i)}_0 \log(1 - \hat{y}_i)$$

The cost is:

$$-\log(\hat{y}_i)$$

Cross Entropy

$$C(\mathbf{w}) = -y_i \log(\hat{y}_i) - (1 - y_i) \log(1 - \hat{y}_i)$$

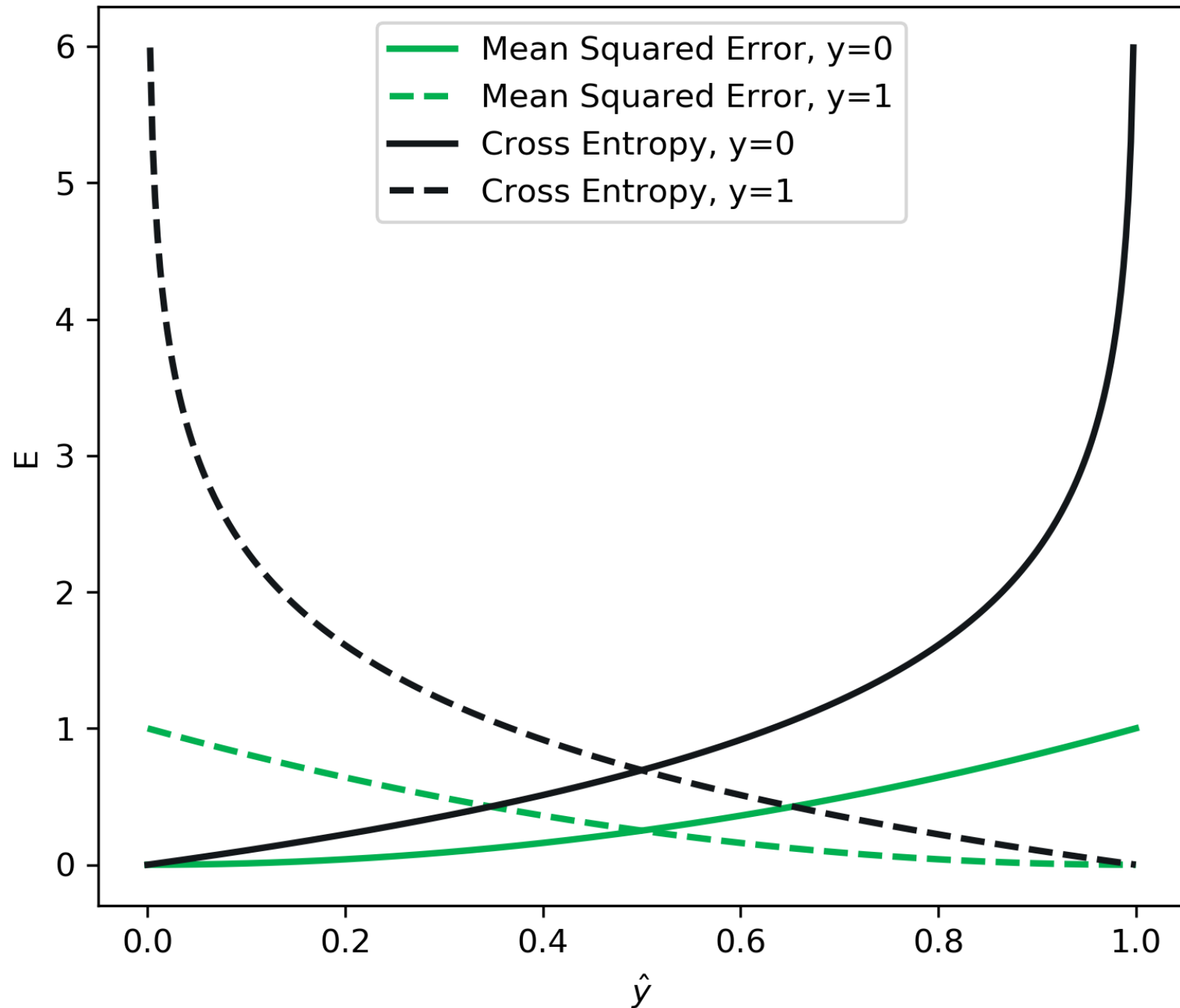
Single sample cost

Target label		Progressively worse predictions →		
CE Cost				
$y_i = 1$	$-\log(\hat{y}_i)$	$\hat{y}_i = 0.4$	$\hat{y}_i = 0.1$	$\hat{y}_i = 0.001$
		$C(\mathbf{w}) = 0.91$	$C(\mathbf{w}) = 2.3$	$C(\mathbf{w}) = 6.9$
$y_i = 0$	$-\log(1 - \hat{y}_i)$	$\hat{y}_i = 0.6$	$\hat{y}_i = 0.9$	$\hat{y}_i = 0.999$
		$C(\mathbf{w}) = 0.91$	$C(\mathbf{w}) = 2.3$	$C(\mathbf{w}) = 6.9$

Cross Entropy vs MSE

If a model is wrong, but is highly confident, it faces exponentially larger penalties with cross-entropy

Cross-entropy as a loss function provides a stronger error penalty for incorrect predictions



Logistic regression does not have a closed-form solution like linear regression did

We need a new approach to optimize the parameters...

Gradient descent

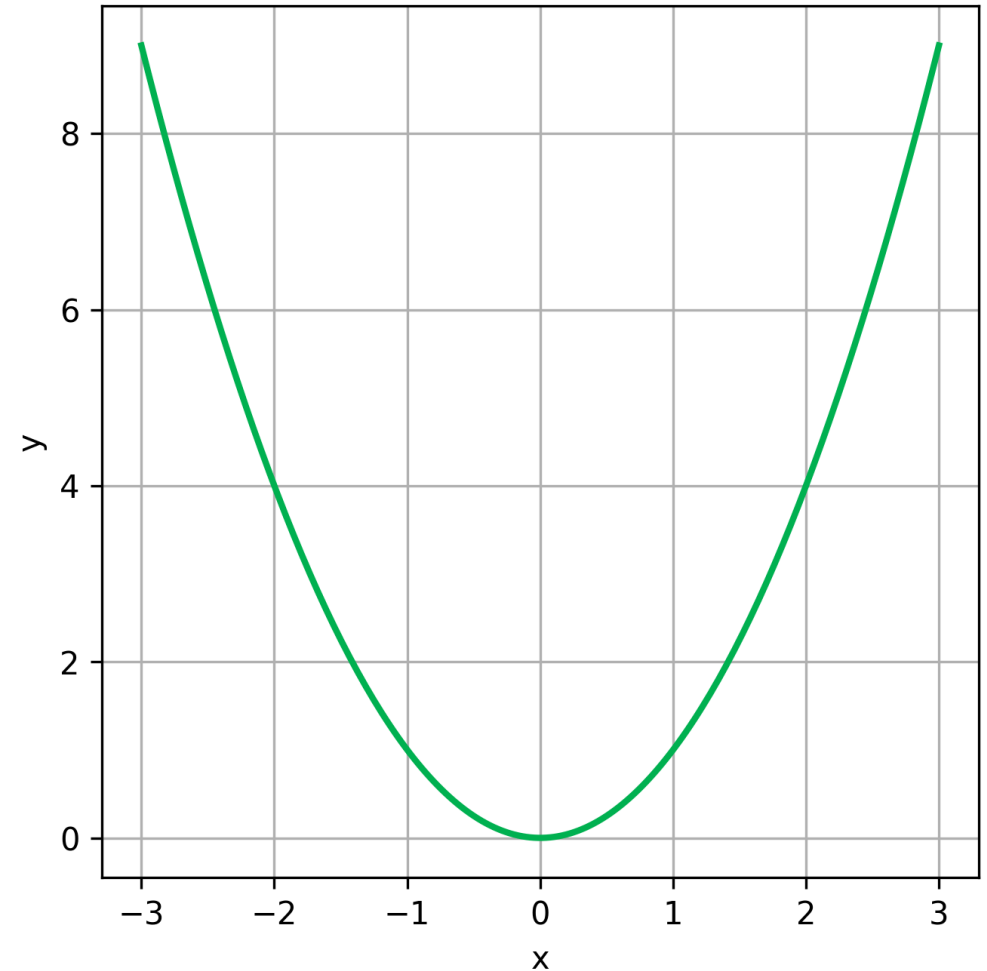
Minimize $y = x^2$

We start at an initial point and want to “roll” down to the minimum

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} + \eta \mathbf{v}$$

Learning
rate

Direction to
move in



Gradient descent

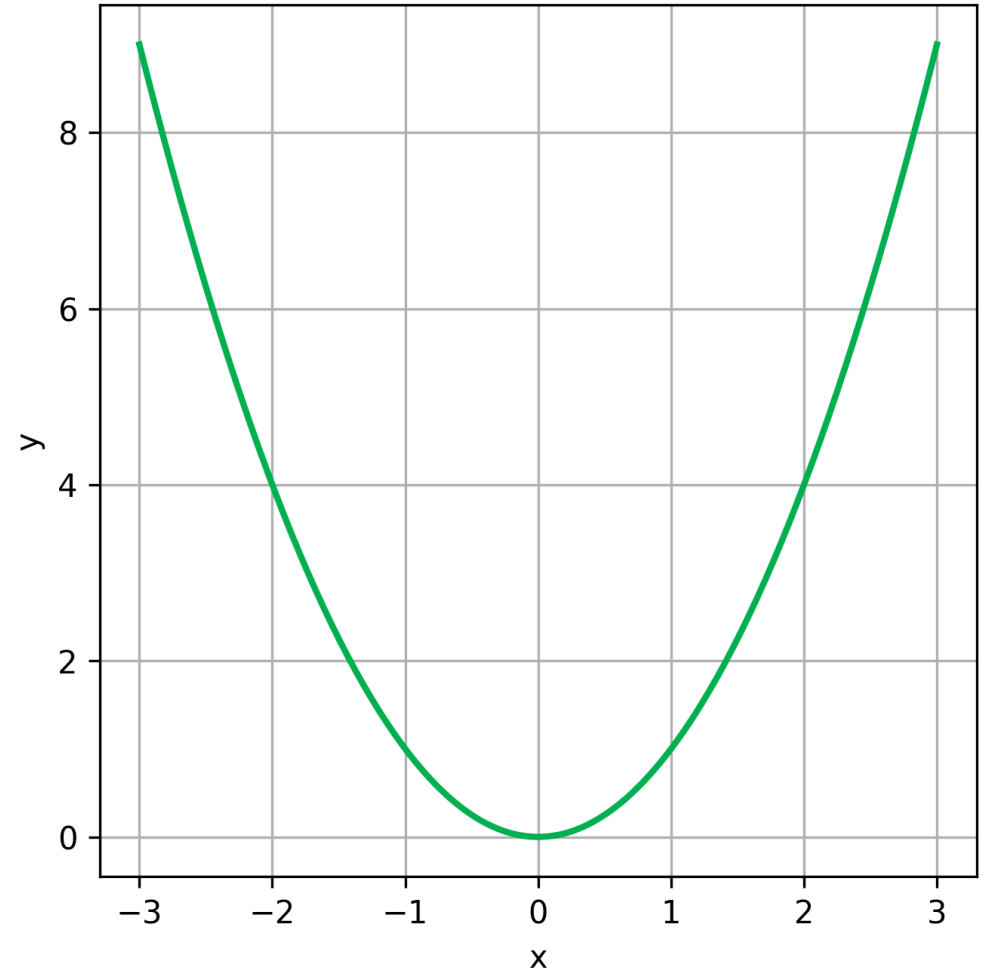
Minimize $f(x) = x^2$

The gradient points in the direction of steepest **positive** change

$$\frac{df(x)}{dx} = 2x$$

We want to move in the **opposite** direction of the gradient

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$$



Gradient descent

Derivative:
$$\frac{df(x)}{dx} = 2x$$

Gradient descent update equation:
$$x^{(i+1)} = x^{(i)} - \eta \nabla f(x^{(i)})$$

Minimize $f(x) = x^2$

Assume $x^{(0)} = 2$ and $\eta = 0.25$

$$x^{(i+1)} = x^{(i)} - (0.25)(2x^{(i)})$$

$$x^{(i+1)} = x^{(i)} - (0.5)x^{(i)}$$

i	$x^{(i)}$	$y^{(i)}$
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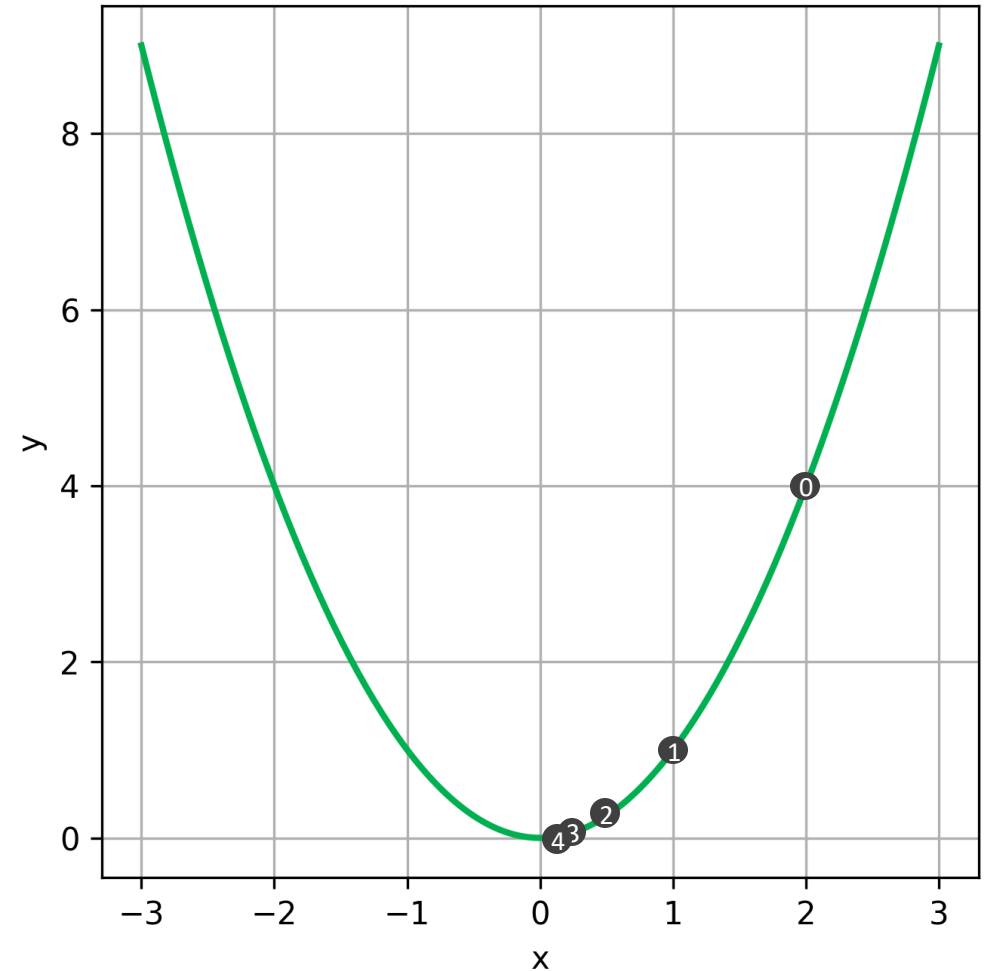
0	2	4
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1	1	1
---	---	---

2	0.5	0.25
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3	0.25	0.0625
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4	0.125	0.0156
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Takeaways

Transformations of features (**feature extraction**) may help to change nonlinear relationships into linear relationships

Logistic regression is suited for classification

For classification problems, we typically apply **cross entropy loss** as the cost function

Logistic regression parameters require a different optimization strategy than OLS; one method for that optimization is **gradient descent**