Linear models II

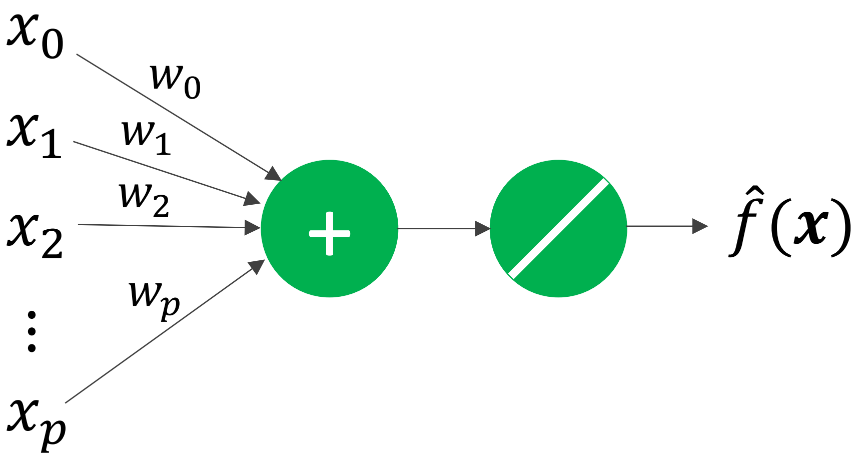
Lecture 07

Quiz

Moving from regression to classification

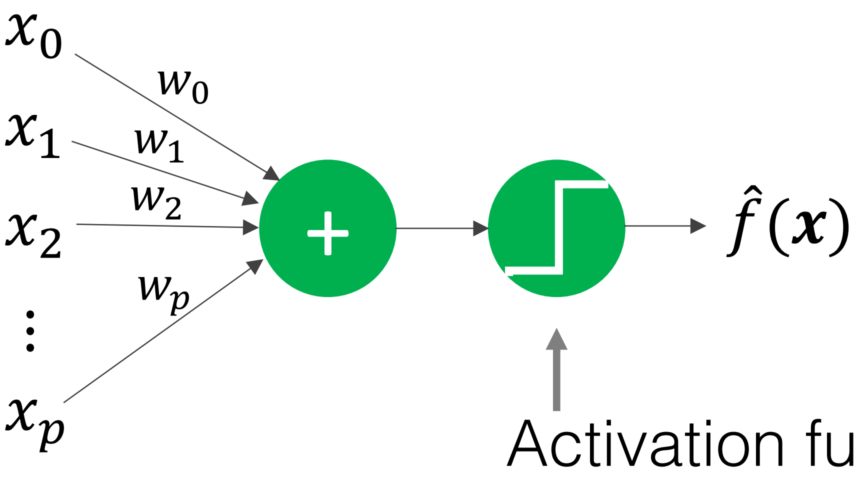
Linear Regression

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



Linear Classification
(perceptron)

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



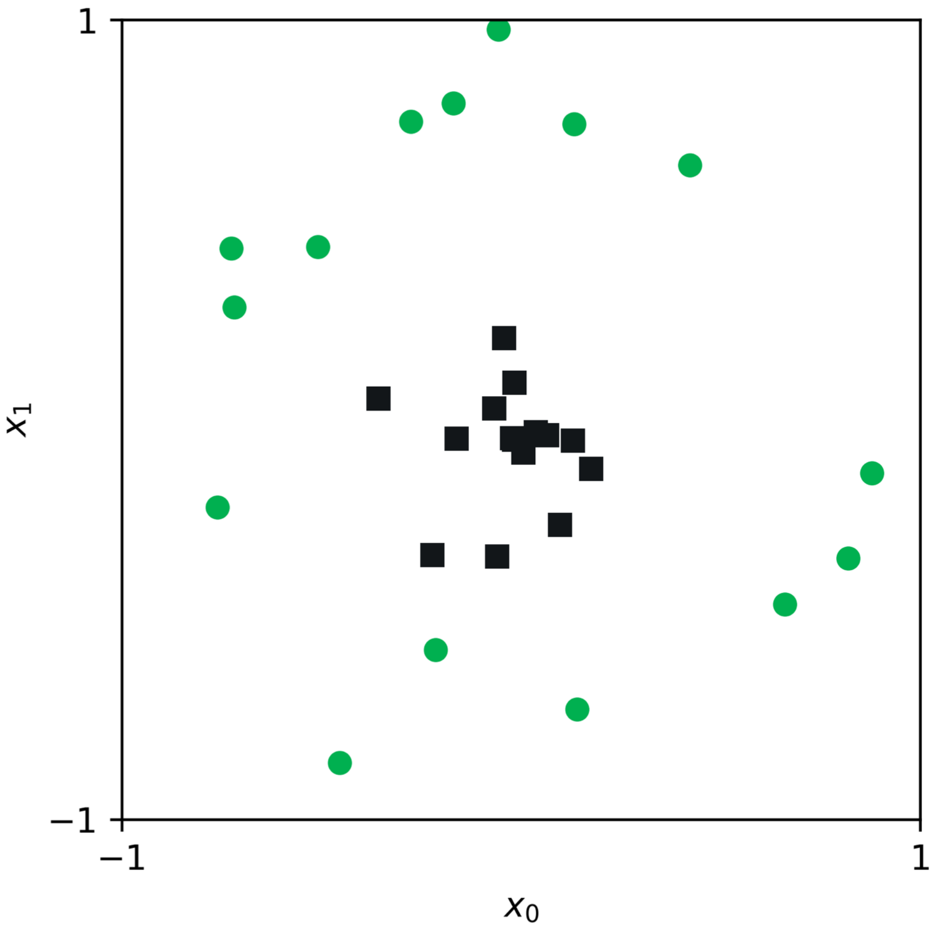
Source: Abu-Mostafa, Learning from Data, Caltech

Can I model nonlinear relationships?

Limitations of linear decision boundaries

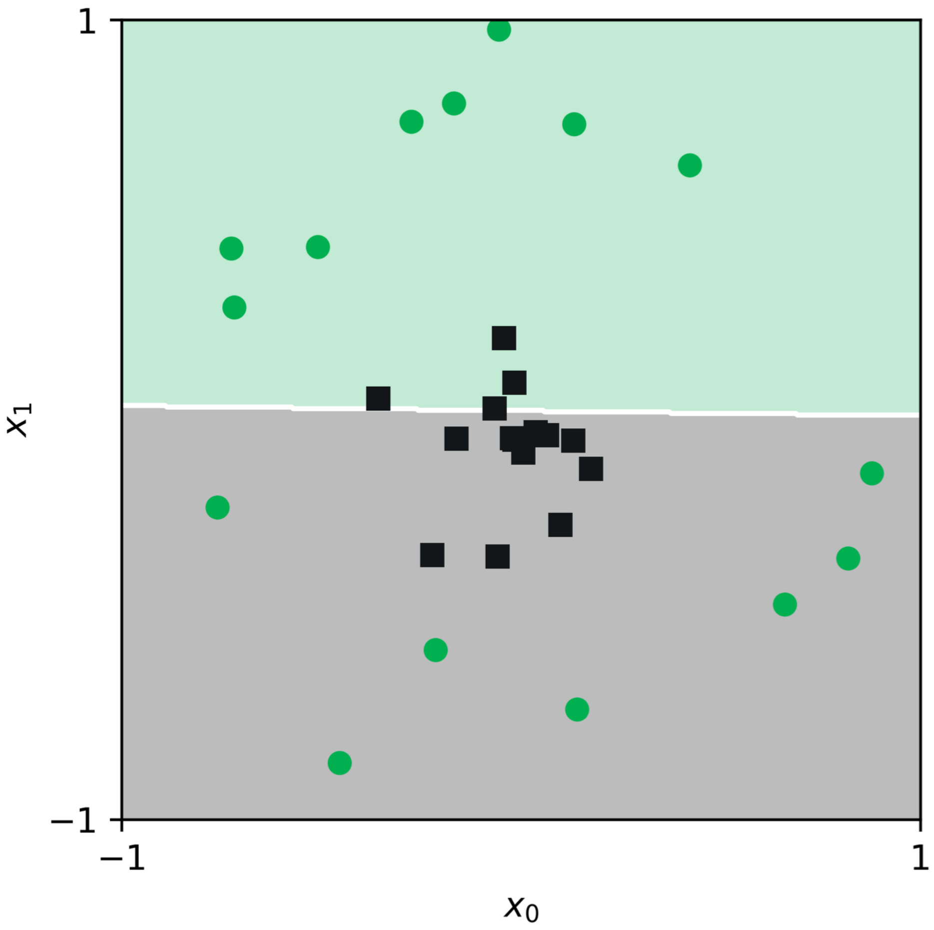
Original data

$\boldsymbol{x}$



Classify the features in this X-space

$\hat{f}_{\boldsymbol{x}}(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{w}^T \boldsymbol{x})$



Transformations of features

Recall our digits example…

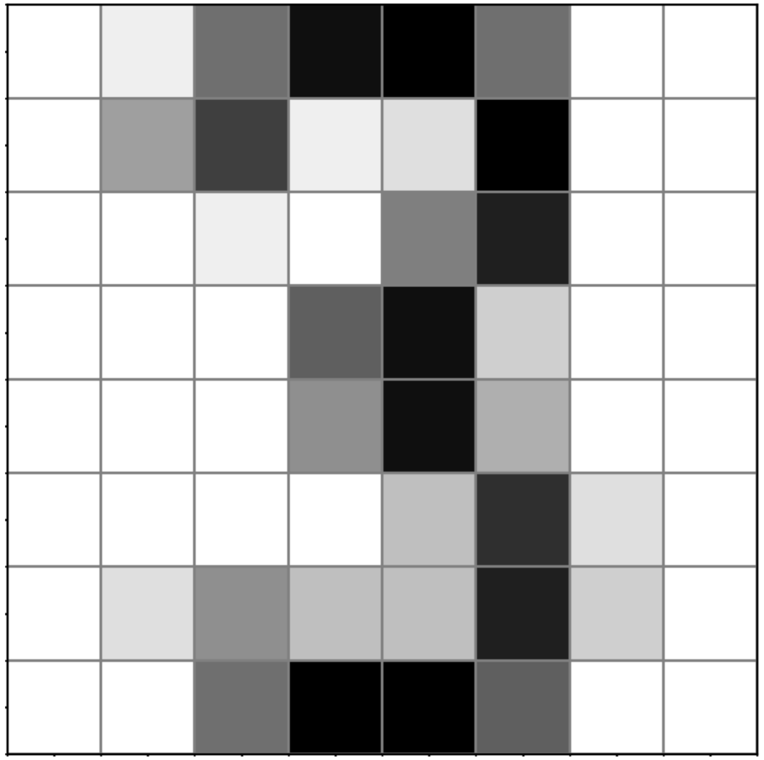
$$\boldsymbol{x} = [x_1, x_2, x_3, \dots, x_{64}]$$

We could create features based on the raw features. For example:

$$\boldsymbol{z} = [x_1 x_2, x_3^2, \frac{x_{64}}{x_{42}}]$$

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

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

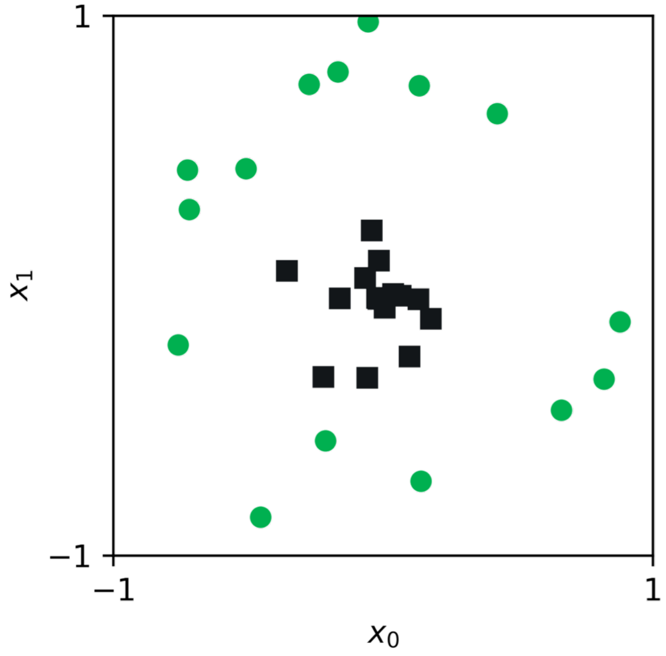


Source: Abu-Mostafa, Learning from Data, Caltech

1

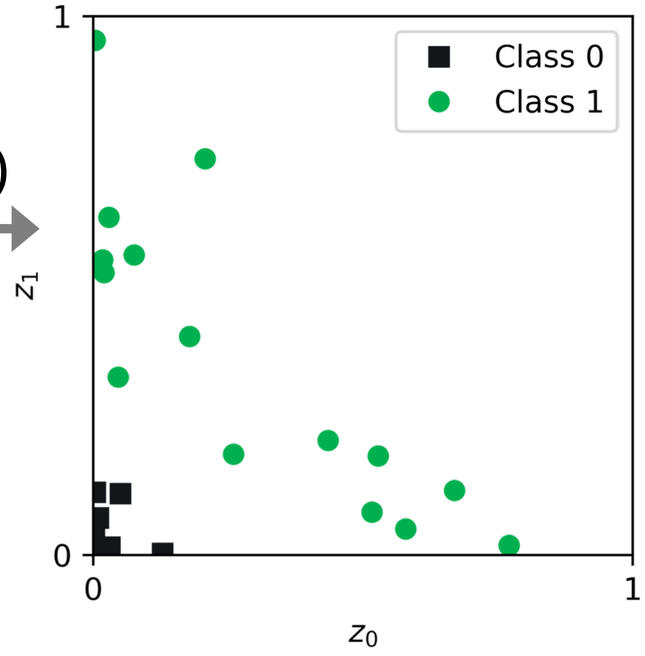
Original data

$\boldsymbol{x}$



transform the data

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



2

This example transform is quadratic

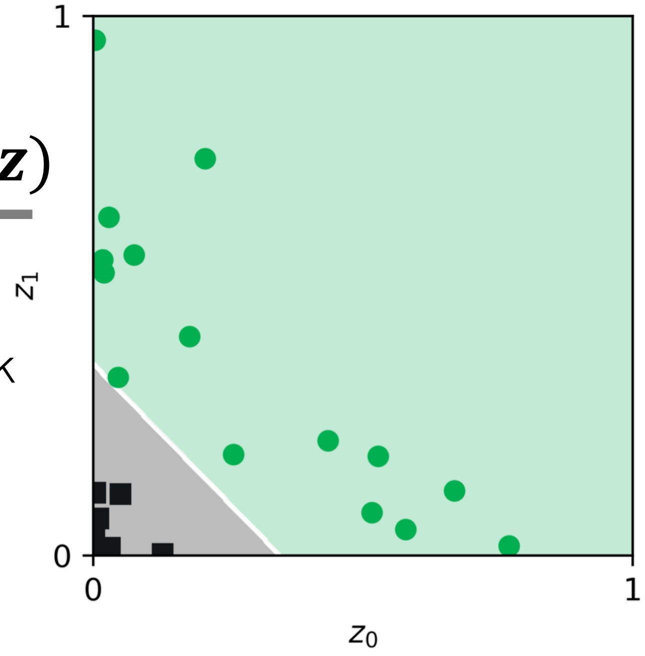
$$z_i = \Phi(x_i) = x_i^2$$

$$z_0 = x_0^2$$

$$z_1 = x_1^2$$

Classify the features in this Z-space

$$\hat{f}_z(\boldsymbol{z}) = \text{sign}(\boldsymbol{w}^T \boldsymbol{z})$$



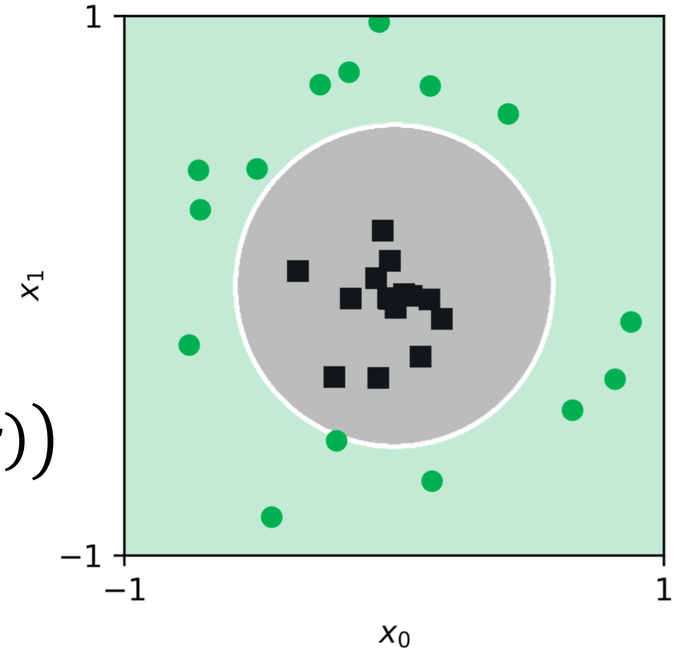
3

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

transform the data back

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

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



Predictions in the original X-space

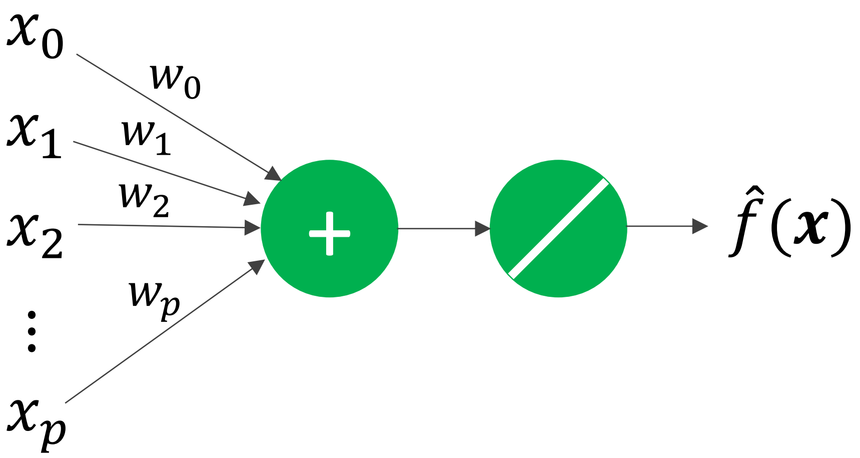
$$\hat{f}(\boldsymbol{x}) = \hat{f}_z(\Phi(\boldsymbol{x}))$$

4

Moving from regression to classification

Linear Regression

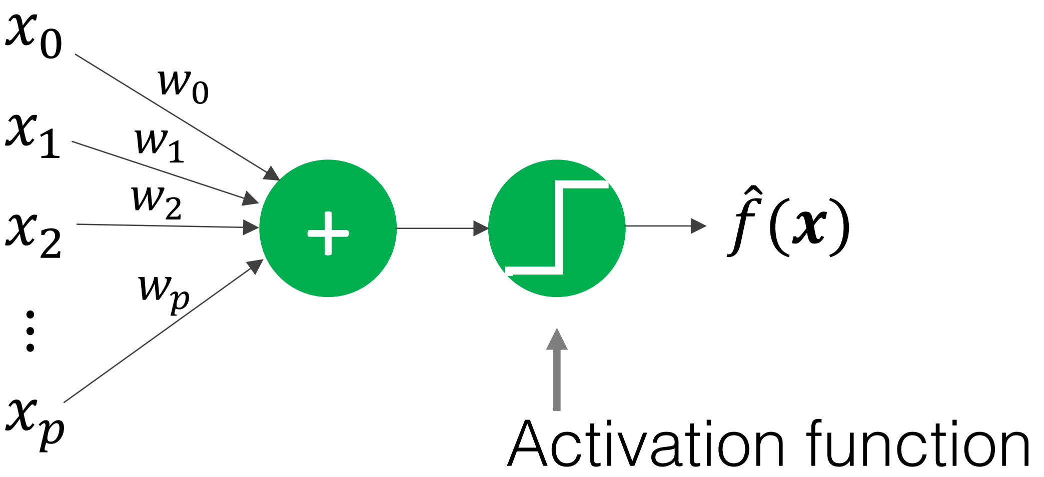
$$\hat{f}(\boldsymbol{x}) = \sum_{i=0}^{p} w_i x_i$$



Linear Classification

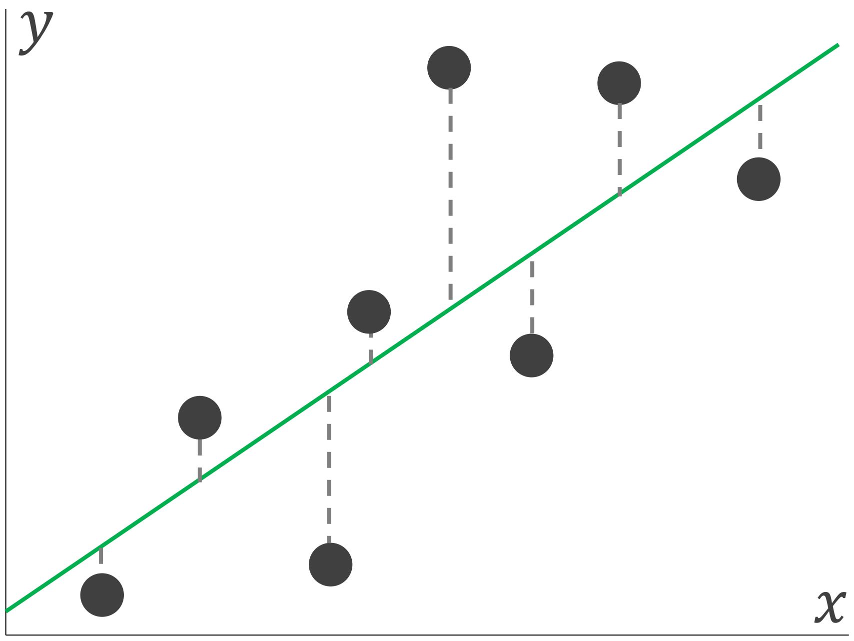
(perceptron)

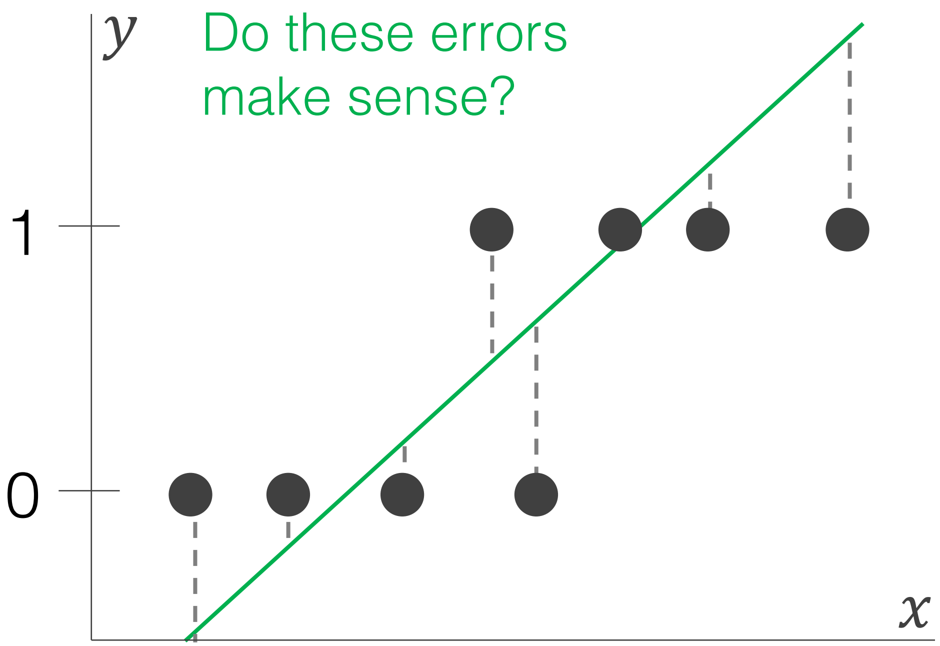
$$\hat{f}(\boldsymbol{x}) = sign\left(\sum_{i=0}^{p} w_i x_i\right)$$



Source: Abu-Mostafa, Learning from Data, Caltech

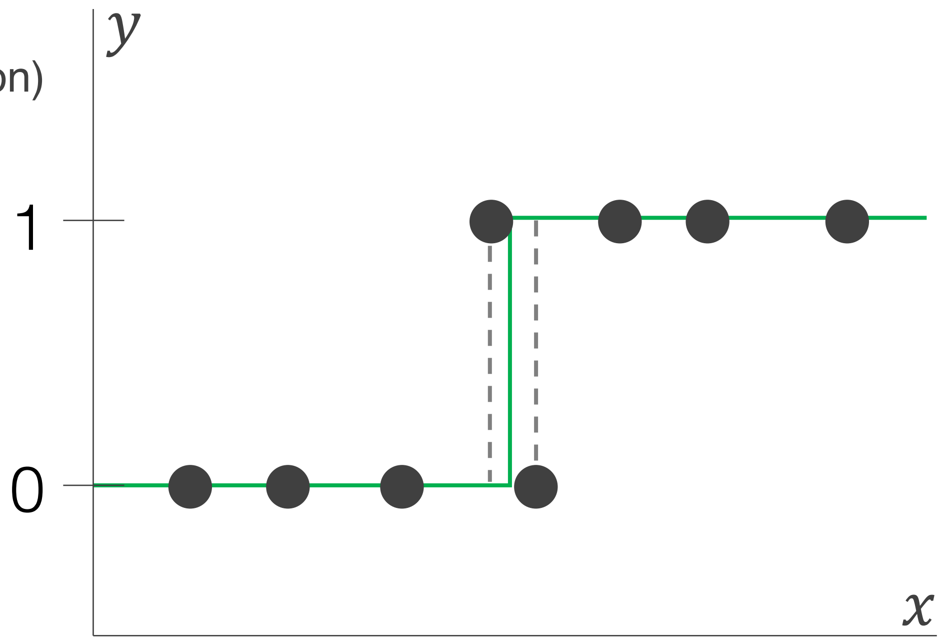
Linear regression

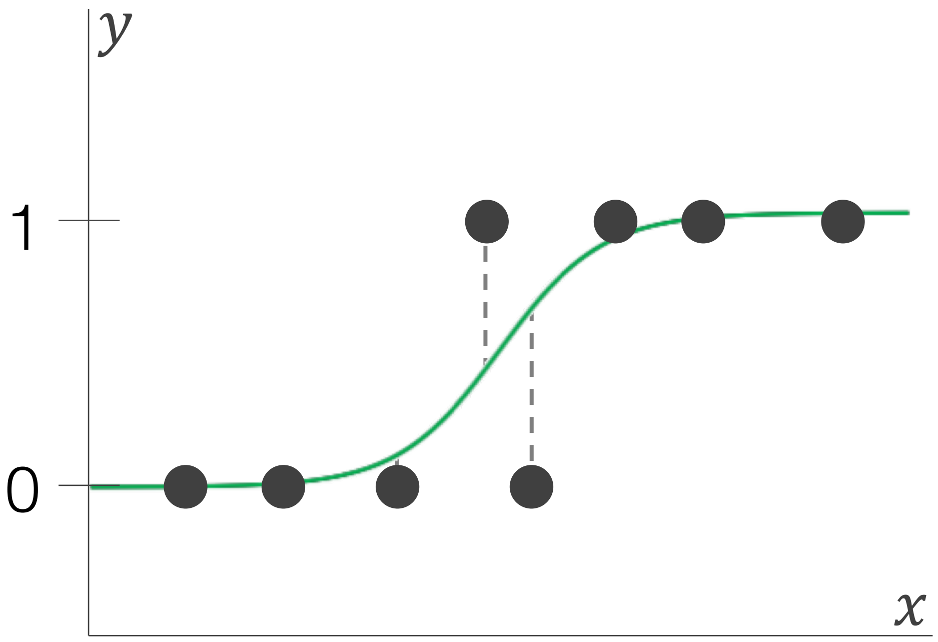




Linear regression applied to a classification problem

Perceptron (sign activation)

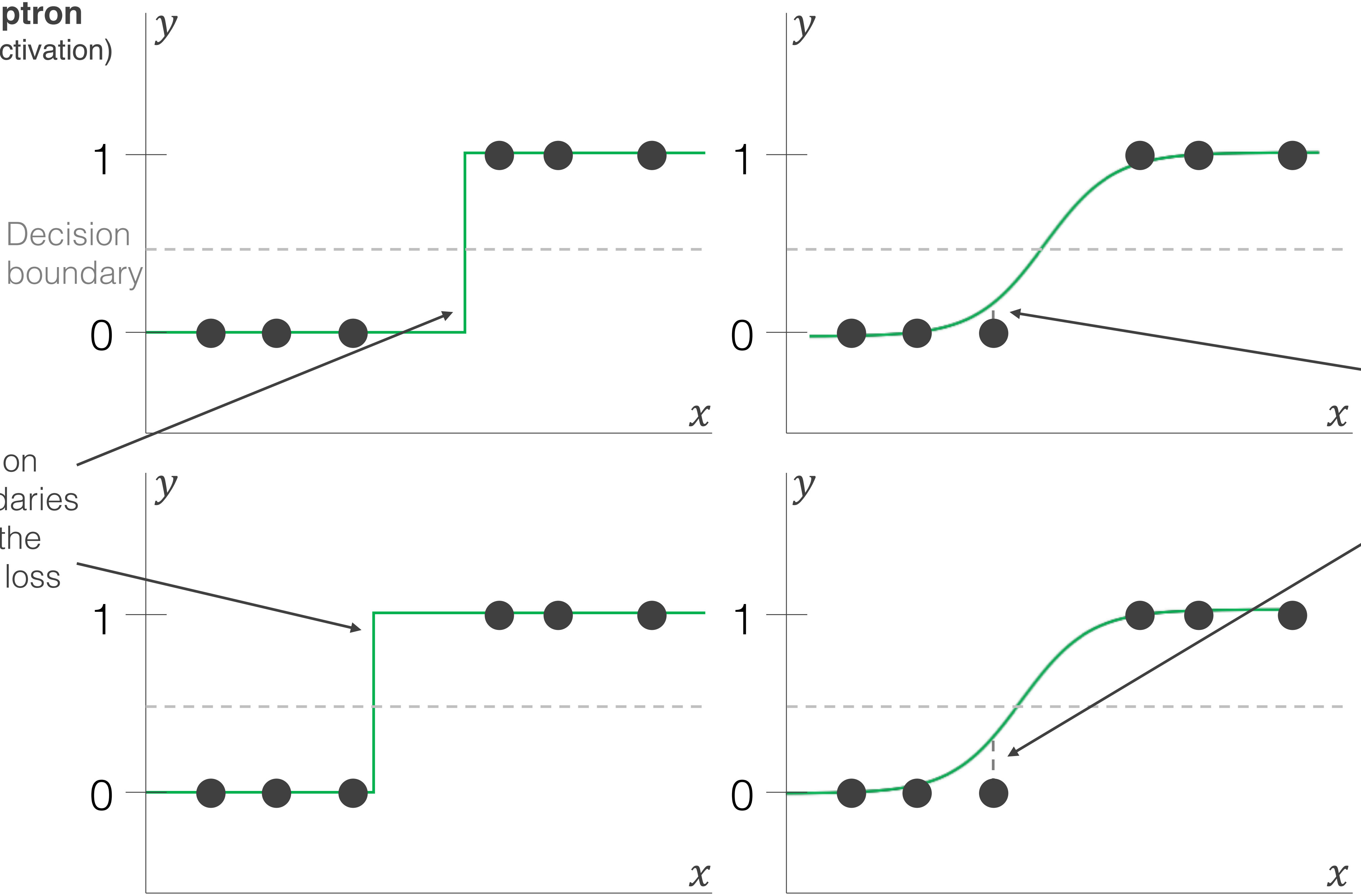




Logistic regression (sigmoid activation)

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

Sigmoid function

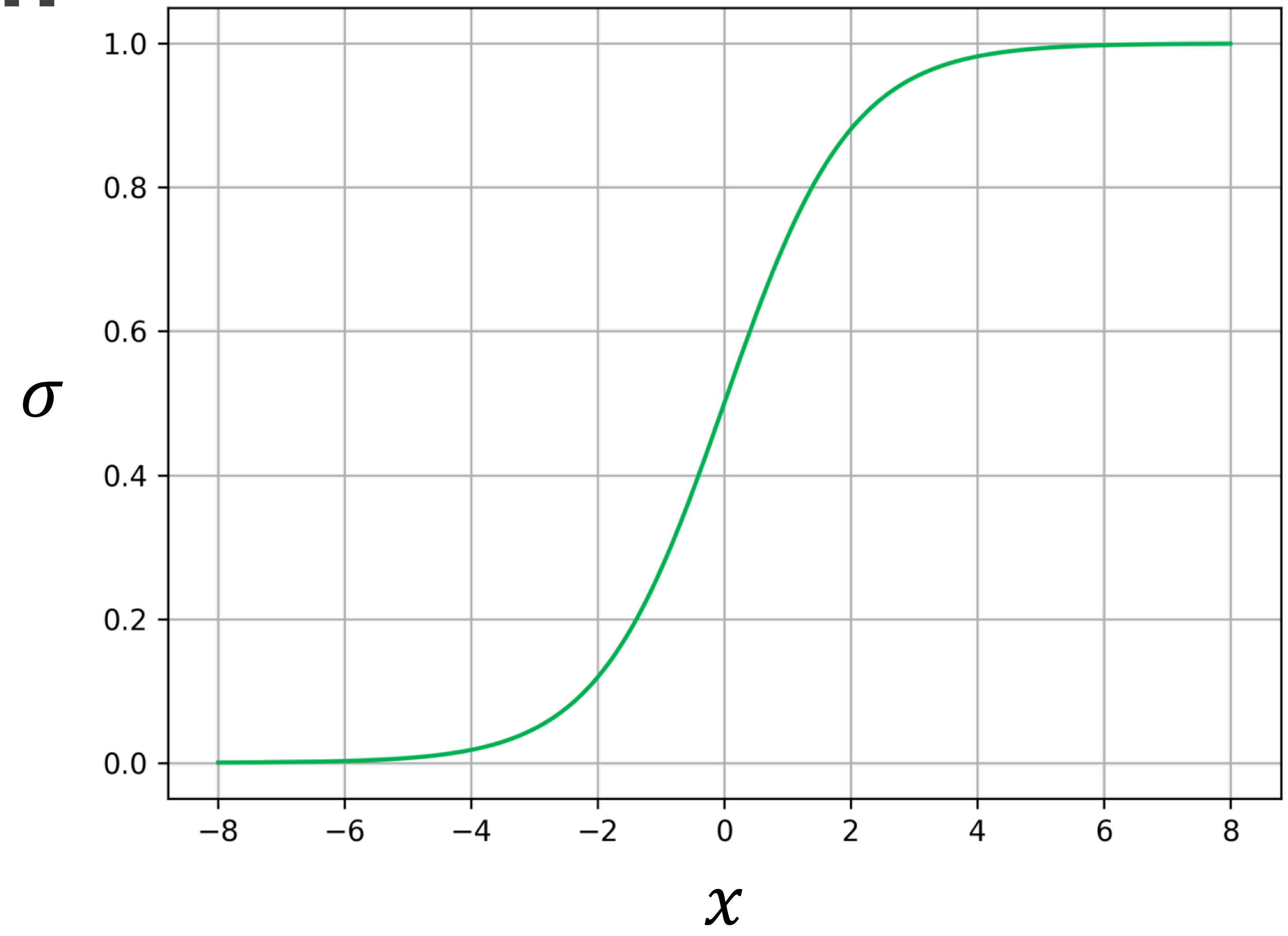
Definition

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

Useful properties

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

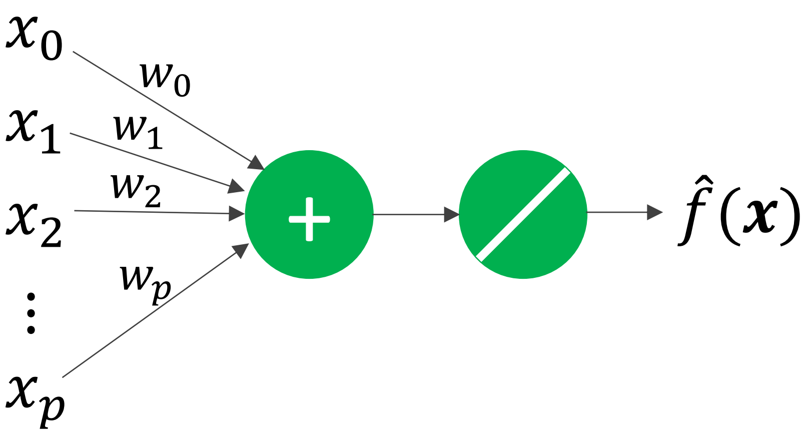
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1-\sigma(x))$$



Moving from regression to classification

Linear Regression

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

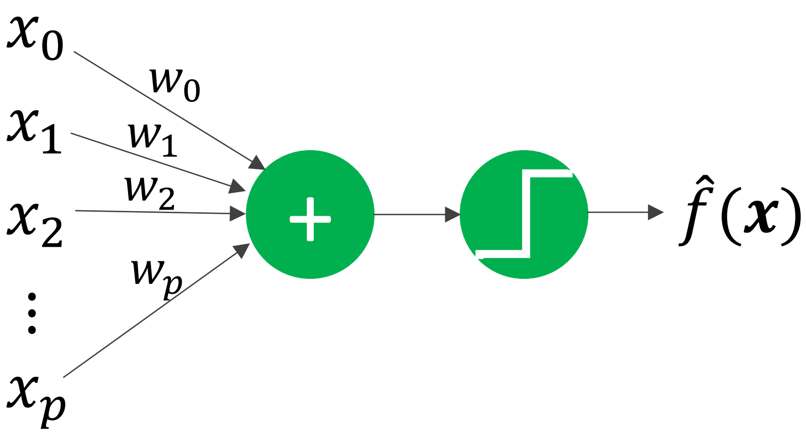


Linear Classification

Perceptron

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

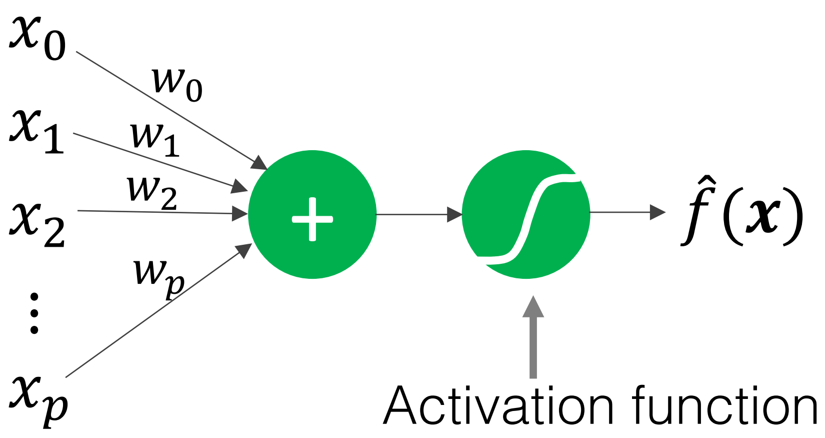
$$sign(x) = \begin{cases} 1 & x > 0 \\ -1 & \text{else} \end{cases}$$



Logistic Regression

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

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



Source: Abu-Mostafa, Learning from Data, Caltech

We take our steps to fitting our model

1. Define a cost function for measuring the fit

2. Optimize the cost function by adjusting model parameters

   a. Calculate the gradient

   b. Set the gradient to zero

   c. Solve for the model parameters

We COULD use the same cost function

Define the previous cost function

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

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

Plug in our model

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

Calculate the gradient

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

Set the gradient to zero and solve for $\boldsymbol{w}$

$$\nabla_w C(\boldsymbol{w}) = \mathbf{0}$$

But we don’t for logistic regression...

There’s a another cost function to use...

Refresher: Maximum Likelihood Estimation

We purchase a bunch of scratch tickets (1,000 of them) and want to determine the probability of them being a winner

Assume we have $N = 1{,}000$ **independent** Bernoulli random variables

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

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

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

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

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

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

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

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

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

$$P(\boldsymbol{x}|p) = p^{\sum x_i}(1-p)^{N-\sum x_i}$$

Maximizing the likelihood is equivalent to maximizing the log-likelihood

$$\ln[P(\boldsymbol{x}|p)] = \ln[p^{\sum x_i}(1-p)^{N-\sum x_i}]$$

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

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

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

$$\frac{\partial \ln[P(\boldsymbol{x}|p)]}{\partial p} = \frac{\sum_{i=1}^{N} x_i}{p} + \frac{N - \sum_{i=1}^{N} x_i}{1-p} = 0$$

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

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

Another interpretation of logistic regression

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

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

Logistic regression models the **probability that features belong to a class**

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

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

The interpretation of the Likelihood

The probability of observing the class labels $y_1, y_2, \dots, y_N$ corresponding to $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N$

The likelihood for **one observation**:

$$P(y_i|\boldsymbol{x}_i) = P(y_i = 1|\boldsymbol{x}_i)^{y_i} P(y_i = 0|\boldsymbol{x}_i)^{1-y_i}$$

The likelihood for **all observations**:

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

Source: Malik Magdon-Ismail, Learning from Data

The likelihood for all observations:

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

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

This is our cost function

(to be precise, the negative of the cost function)

We can take the logarithm, then the gradient, then set equal to zero…

This is not solvable in closed form: need a new approach

Gradient descent

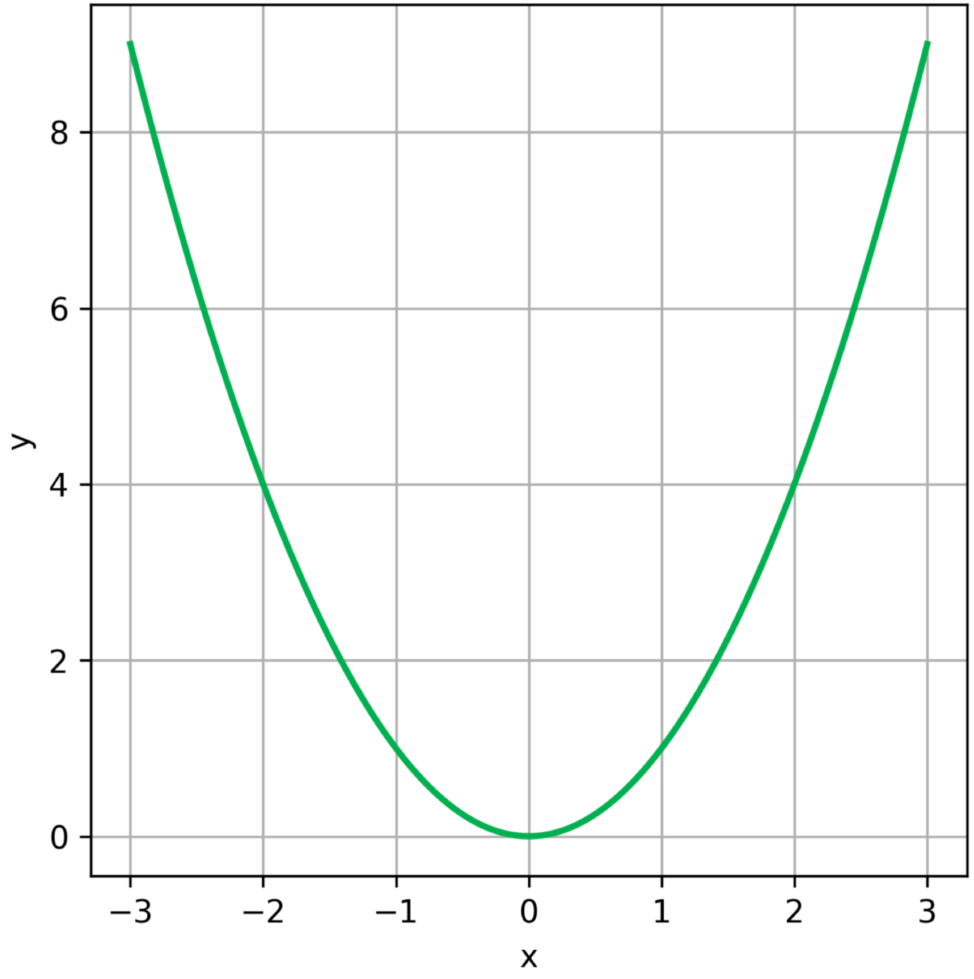
Minimize $y = x^2$

We start at a point and want to "roll" down to the minimum

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

Learning rate

Direction to move in



Gradient descent

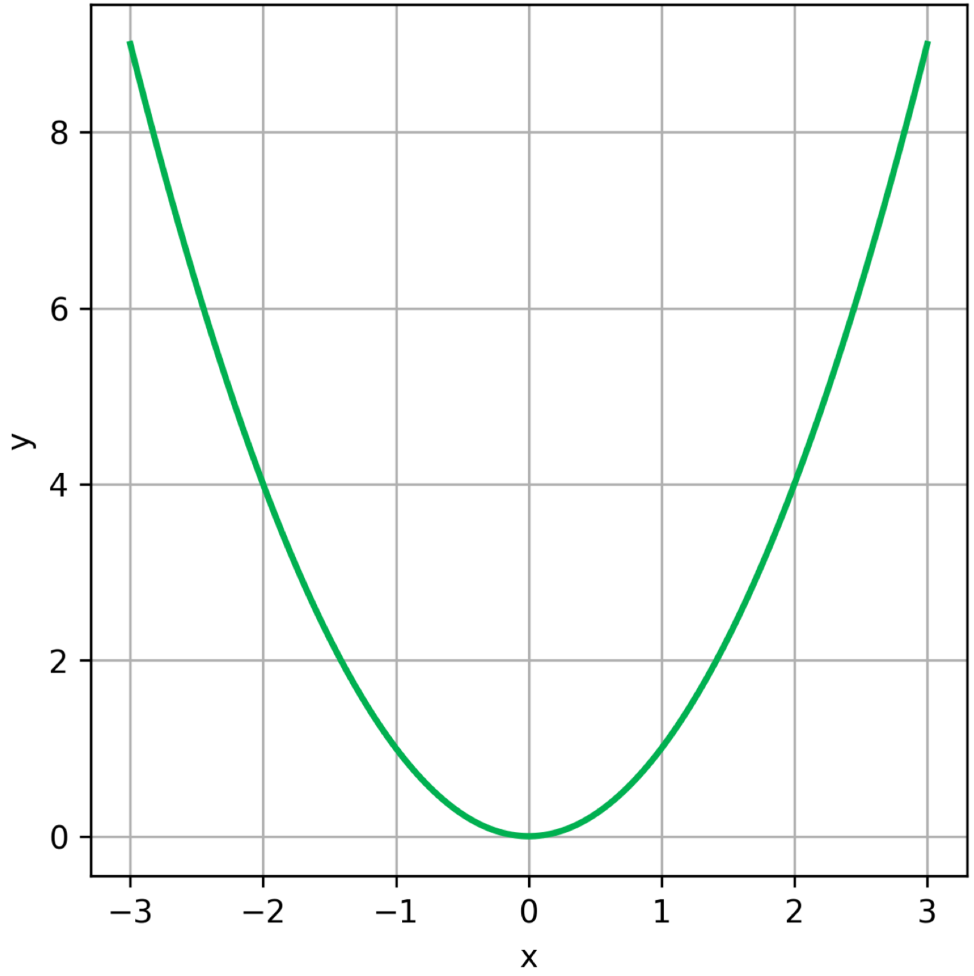
Minimize $f(x) = x^2$

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

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



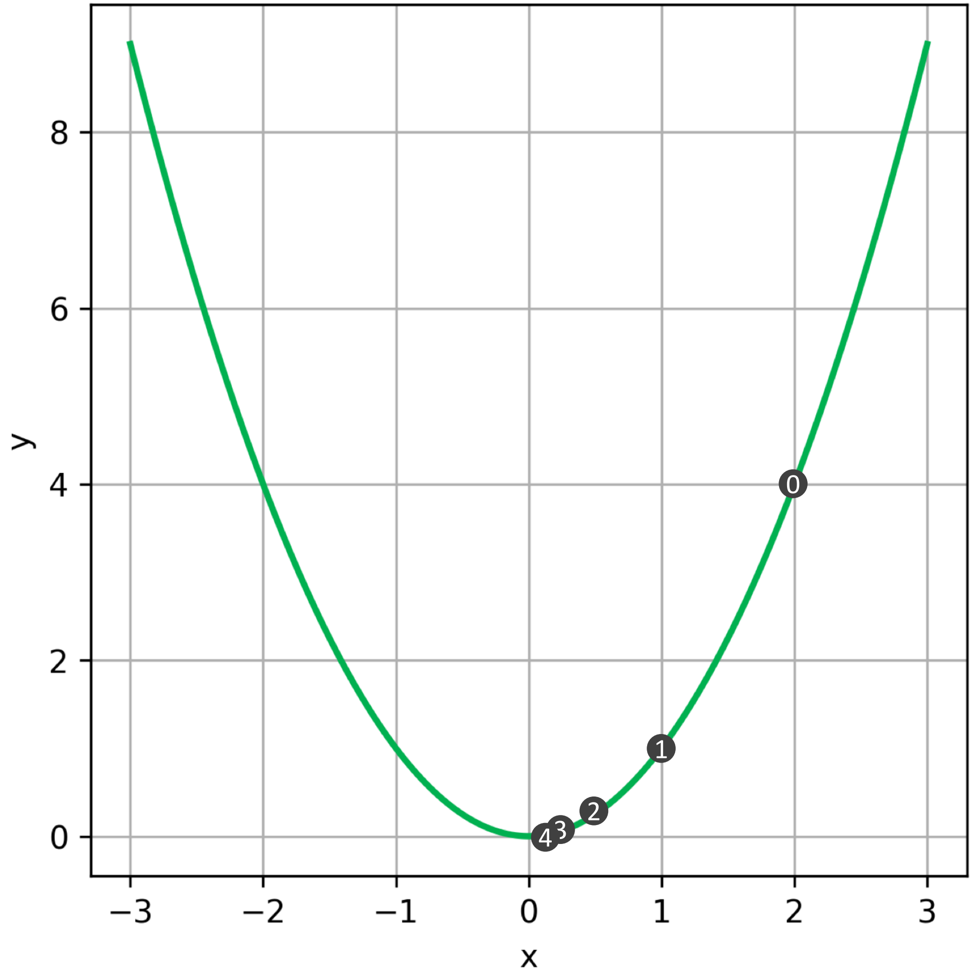
Gradient descent

Minimize $f(x) = x^2$

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

$$\boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} - (0.25)(2\boldsymbol{x}^{(i)})$$
$$\boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} - (0.5)\boldsymbol{x}^{(i)}$$

i	$x^{(i)}$	$y^{(i)}$
0	2	4
1	1	1
2	0.5	0.25
3	0.25	0.0625
4	0.125	0.0156



Takeaways

- Transformations of features may help to overcome nonlinearities
- Logistic regression is much better suited for classification than linear regression
- Logistic regression parameters must be estimated iteratively, and a method for that optimization is gradient descent
- Gradient descent can be used for cost function optimization and there are a number of variants