Linear models II

Lecture 07

Quiz

Moving from regression to classification

Linear Regression

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

Linear Classification

(perceptron)

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

Source: Abu-Mostafa, Learning from Data, Caltech

Moving from regression to classification

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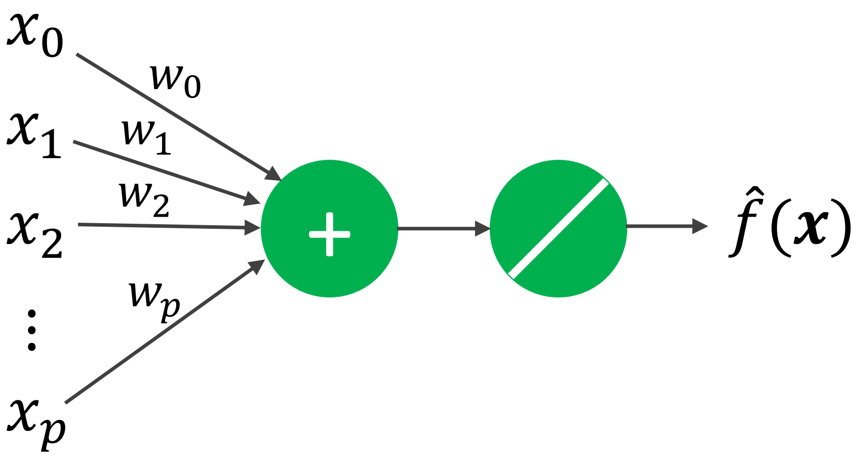

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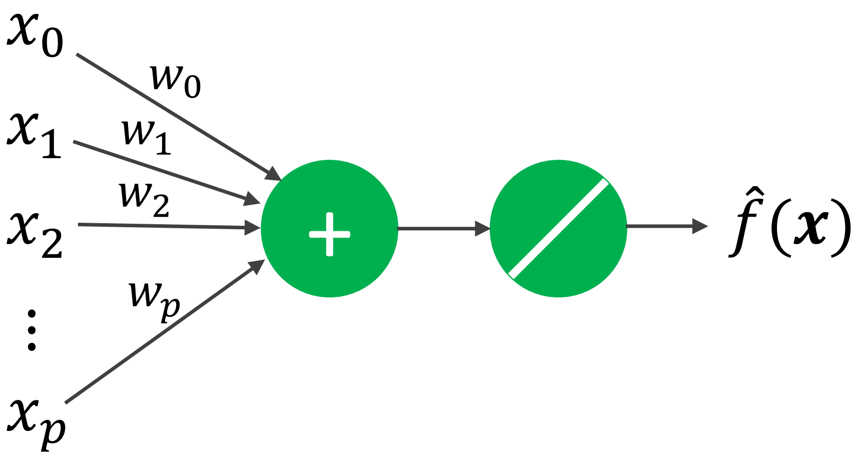

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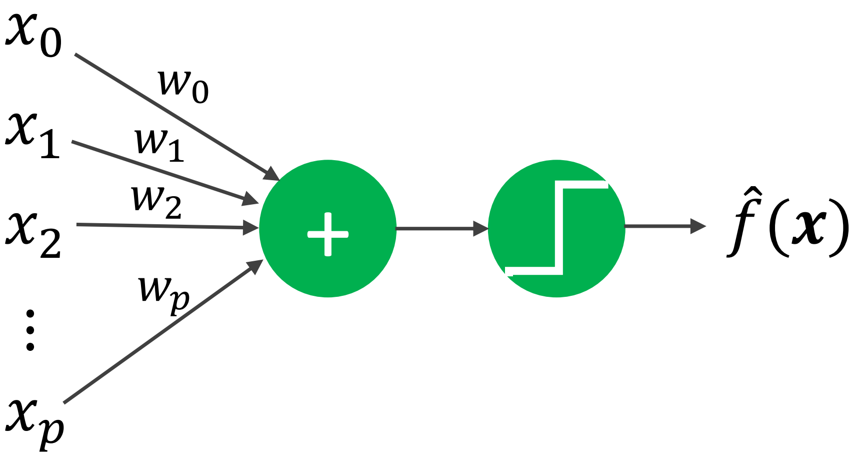

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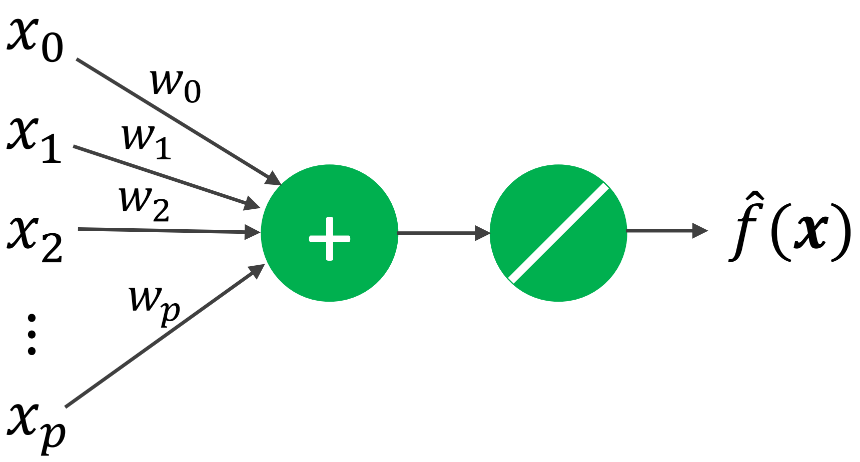

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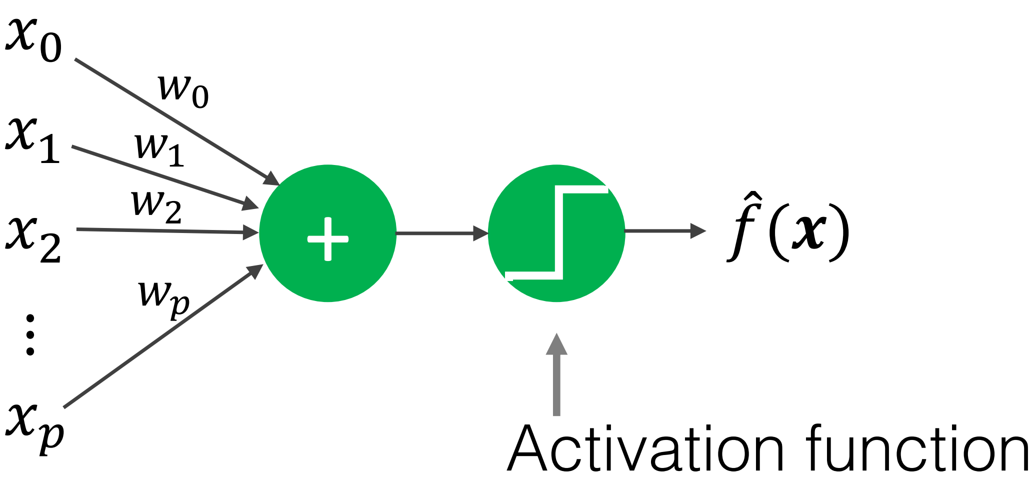


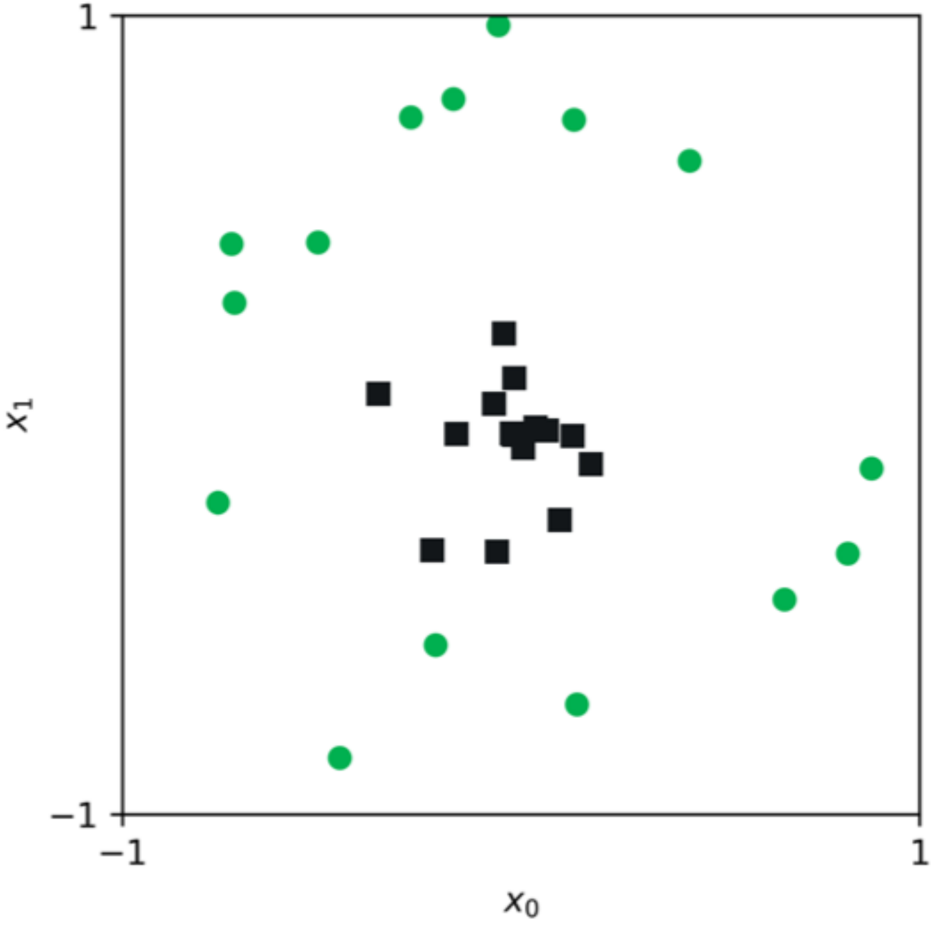
Source: Abu-Mostafa, Learning from Data, Caltech

Can I model nonlinear relationships?

Limitations of linear decision boundaries

Original data

$\boldsymbol{x}$



Limitations of linear decision boundaries

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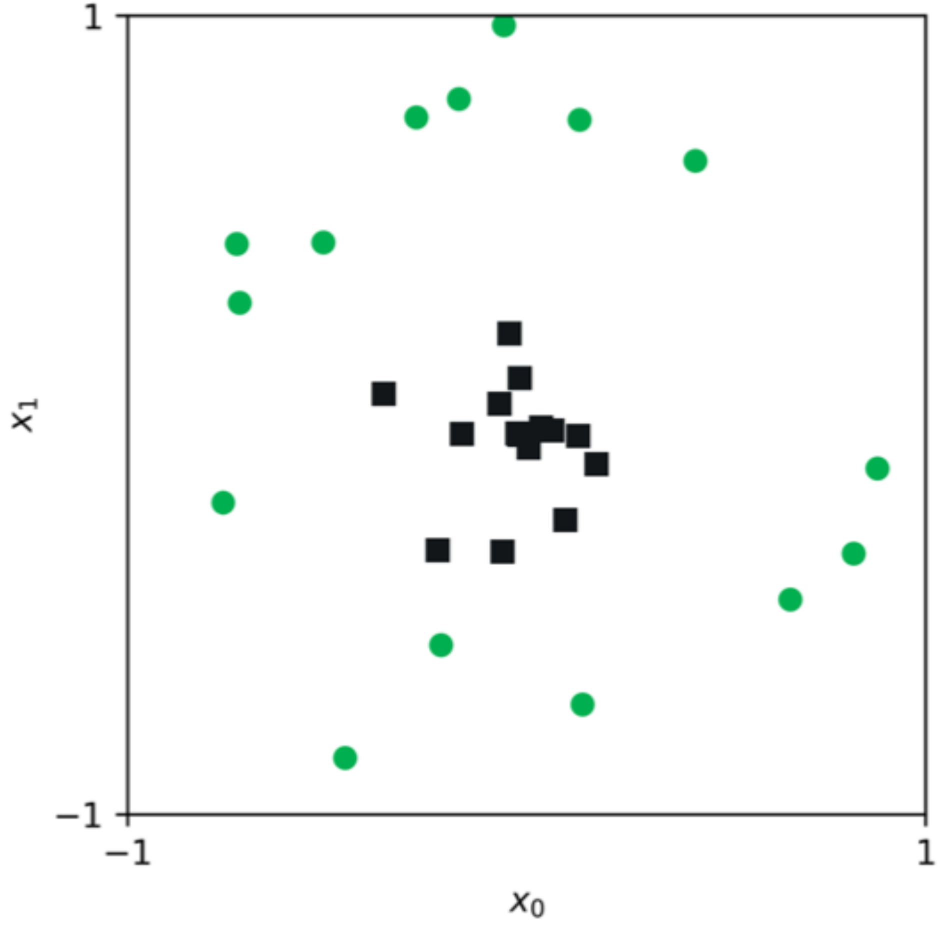
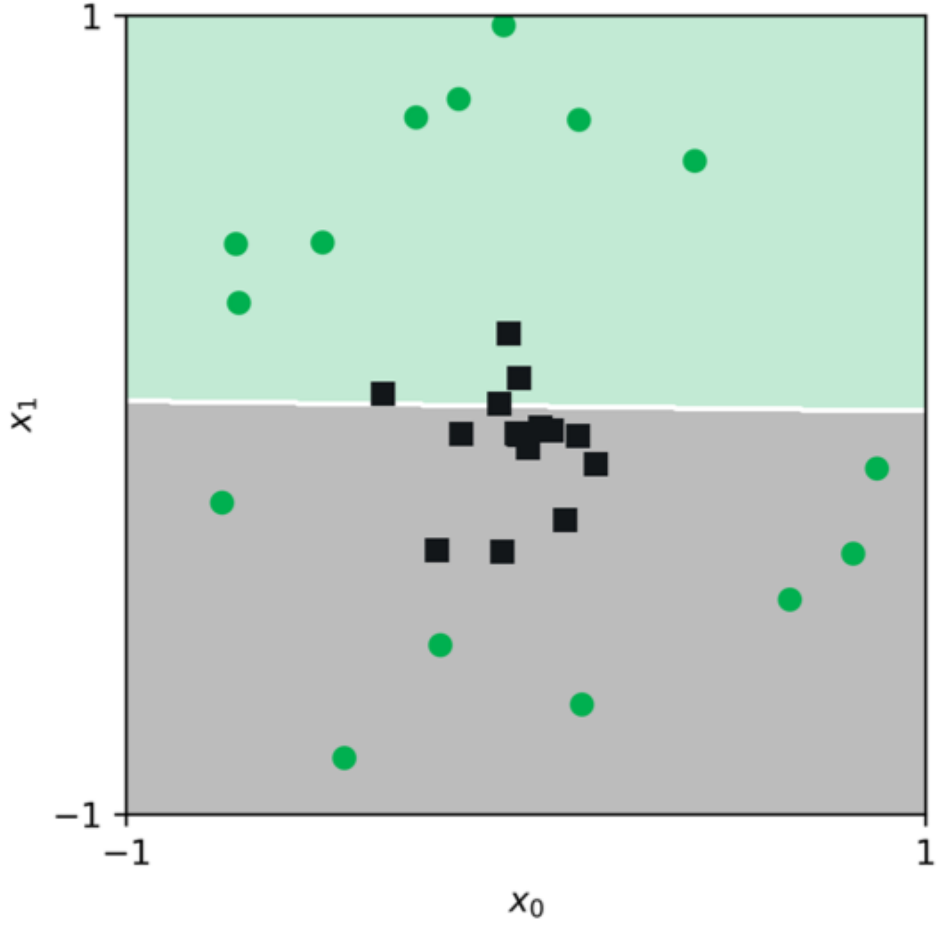


Classify the features in this X-space

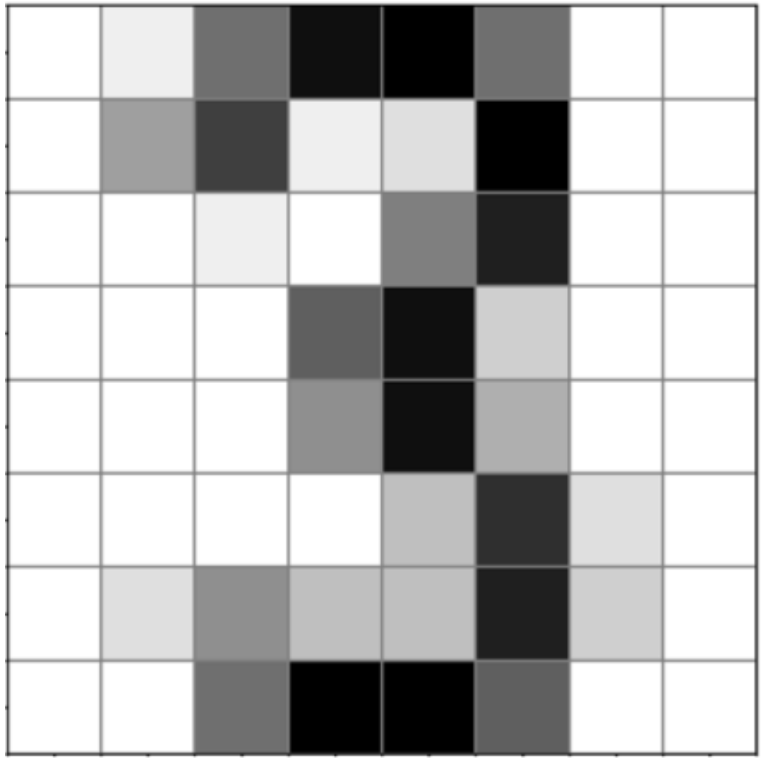
$$\hat{f}_x(\boldsymbol{x}) = \text{sign}(\boldsymbol{x}^T \boldsymbol{z})$$



Transformations of features

Recall our digits example…

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



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Transformations of features

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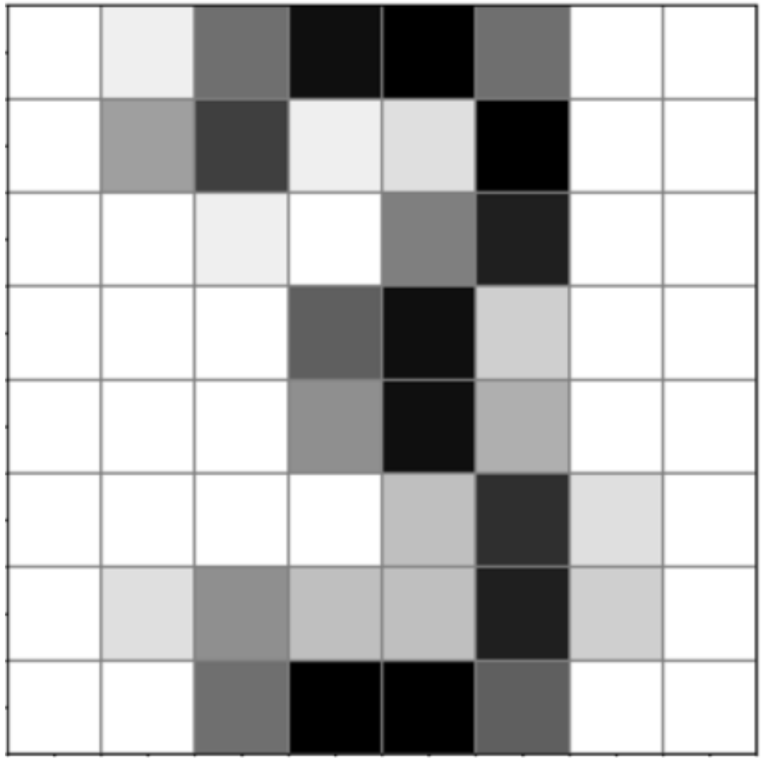
We could create features based on the raw features. For example:

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



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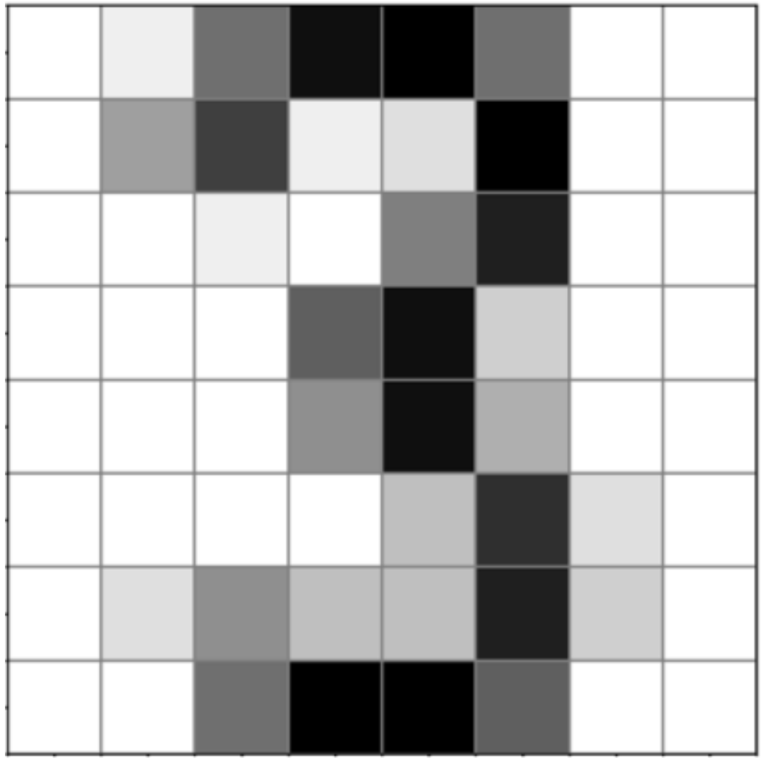
Which can be written simply as variables in a new feature space:

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

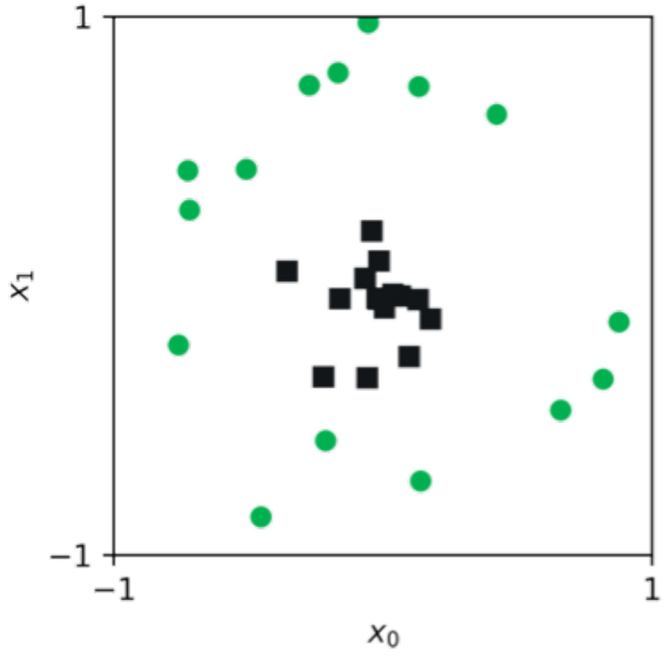


Source: Abu-Mostafa, Learning from Data, Caltech

1

Original data

$\boldsymbol{x}$

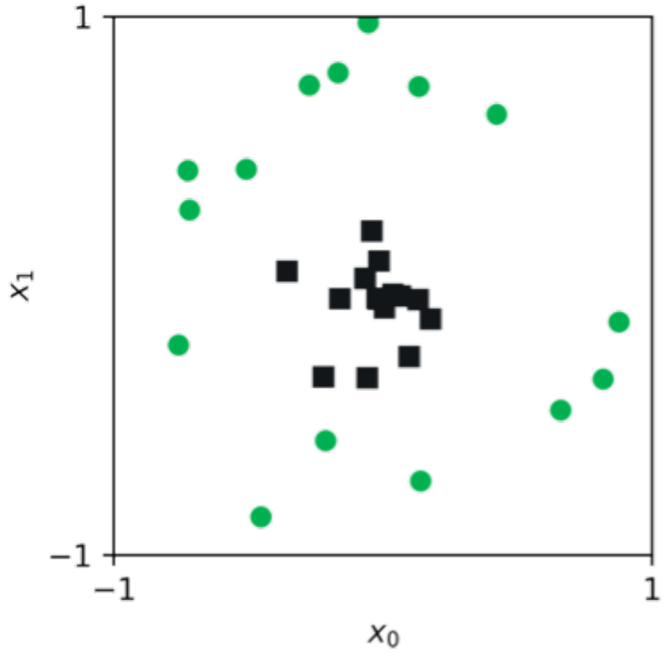


3

1

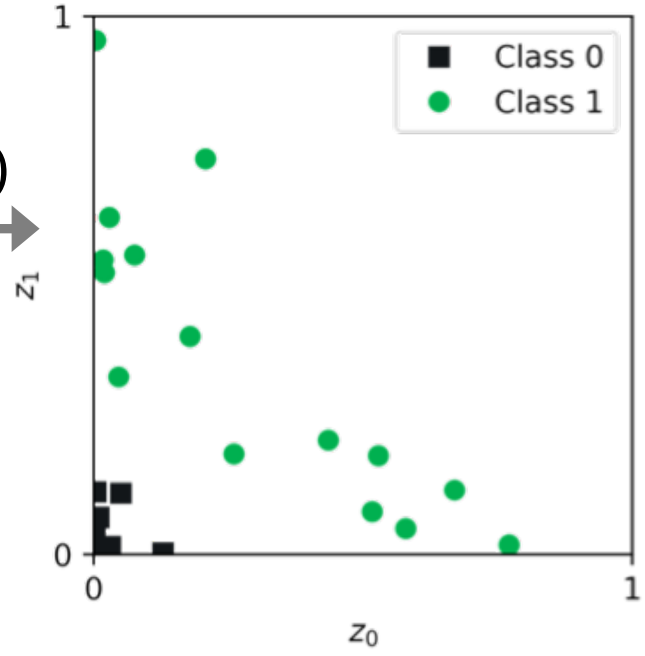
Original data

$\boldsymbol{x}$



transform
the data

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



2

This example transform is quadratic

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

$$z_0 = x_0^2$$

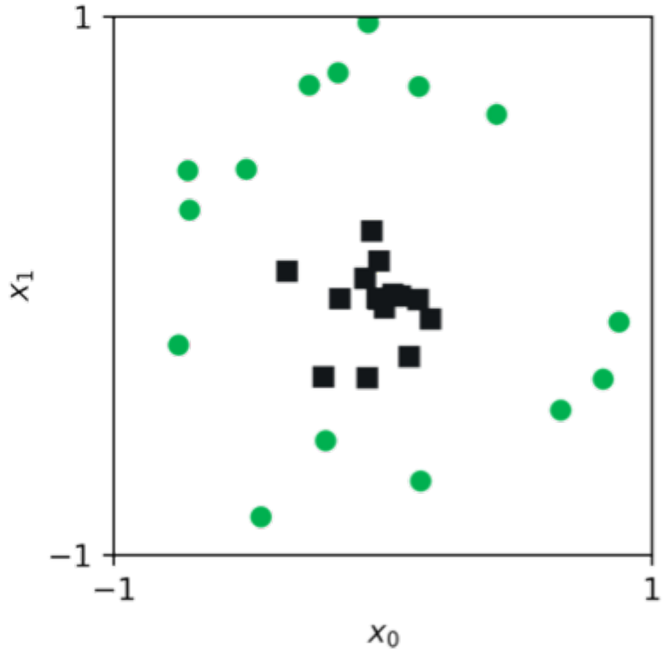
$$z_1 = x_1^2$$

3

1

Original data

$\boldsymbol{x}$



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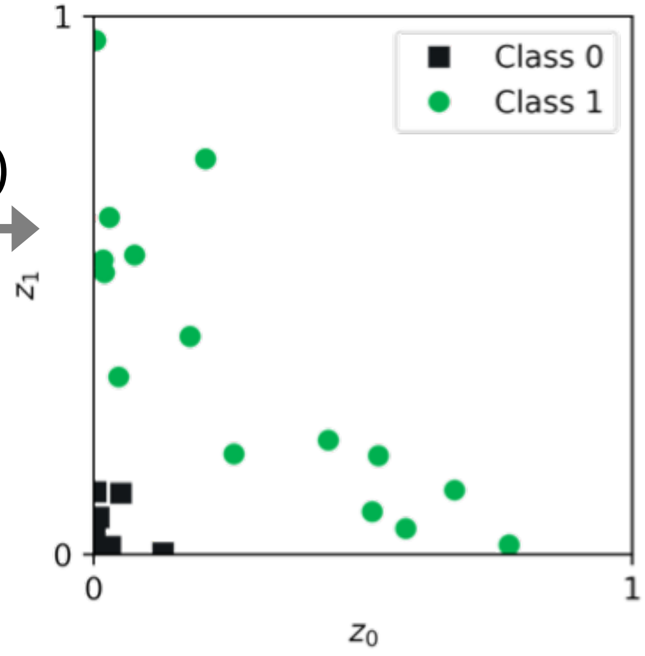

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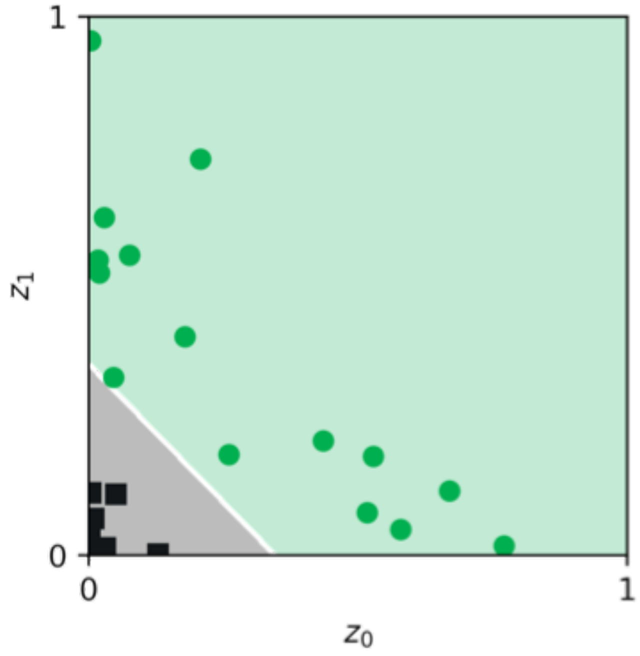
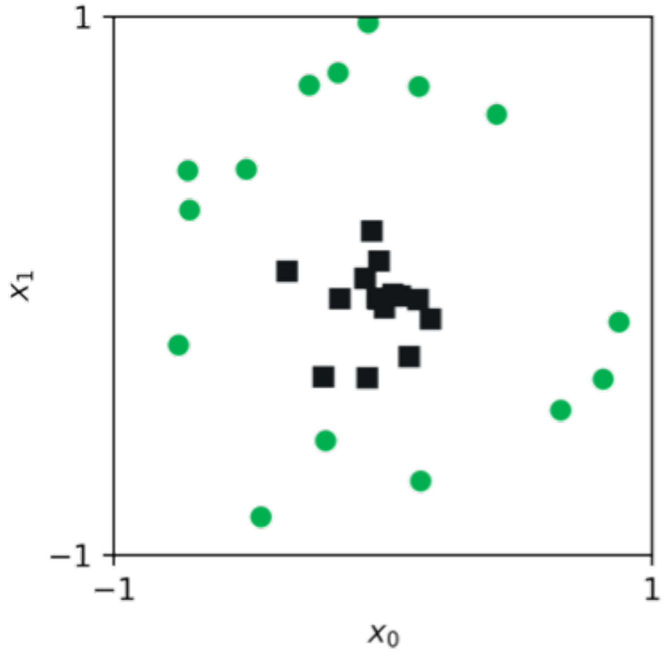


3

1

Original data

$\boldsymbol{x}$



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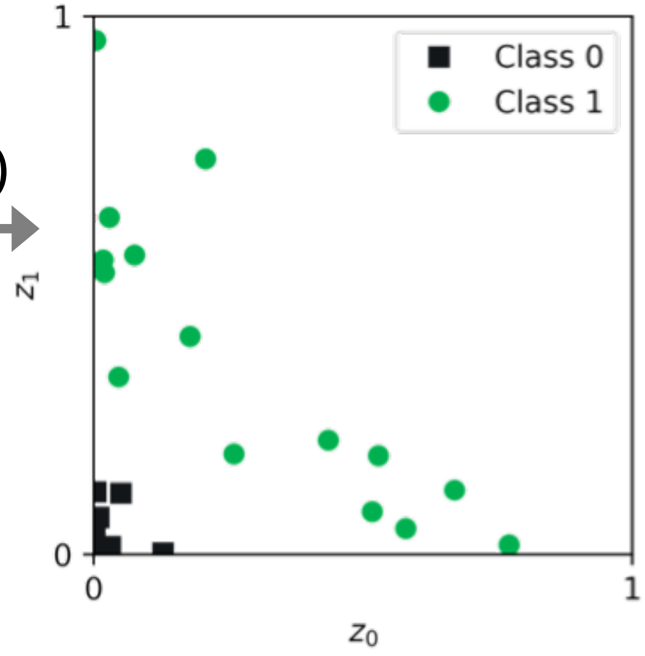

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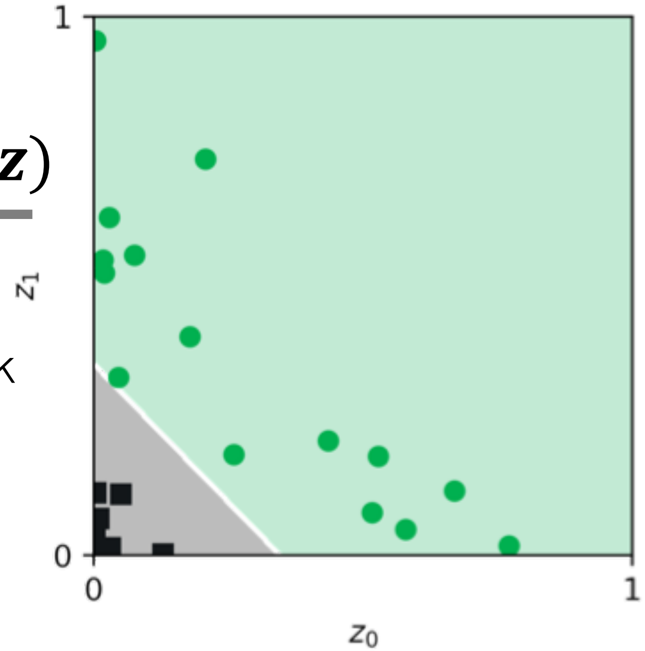


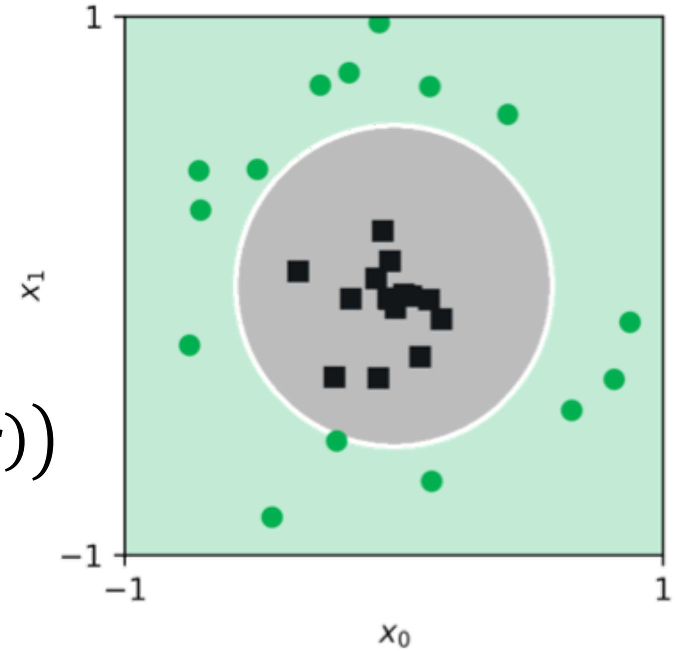
3

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

transform the data back

$x_0 = z_0^{1/2}$

$x_1 = z_1^{1/2}$



Predictions in the original X-space

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

4

Moving from regression to classification

Linear Regression

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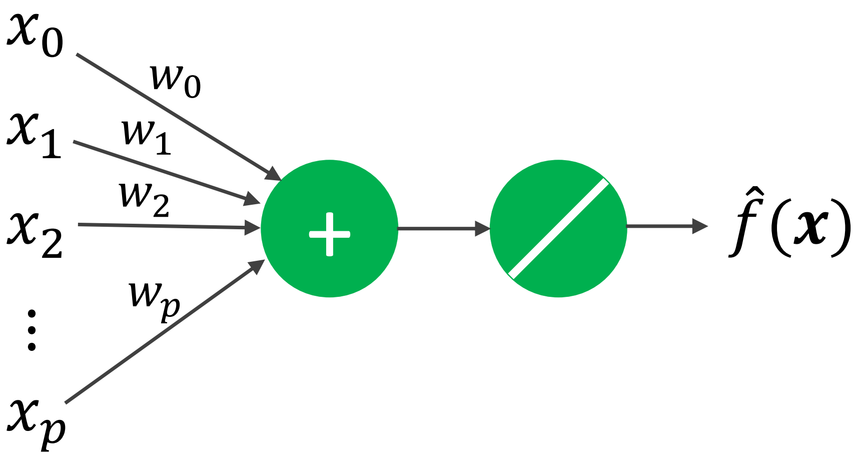

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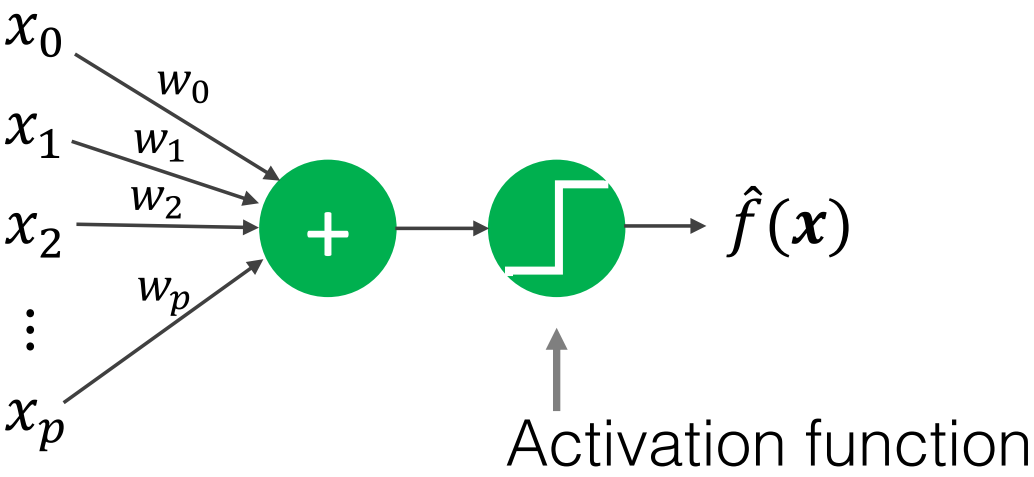
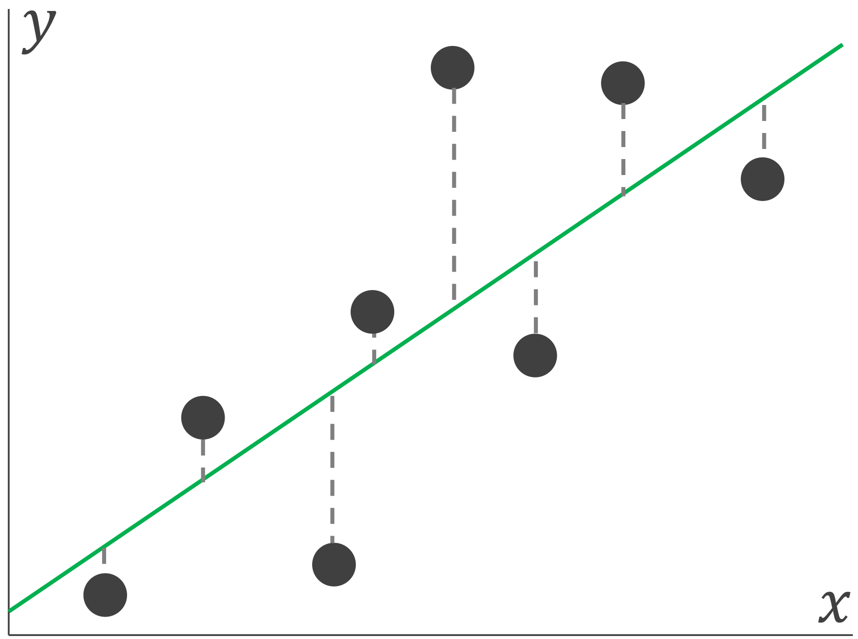
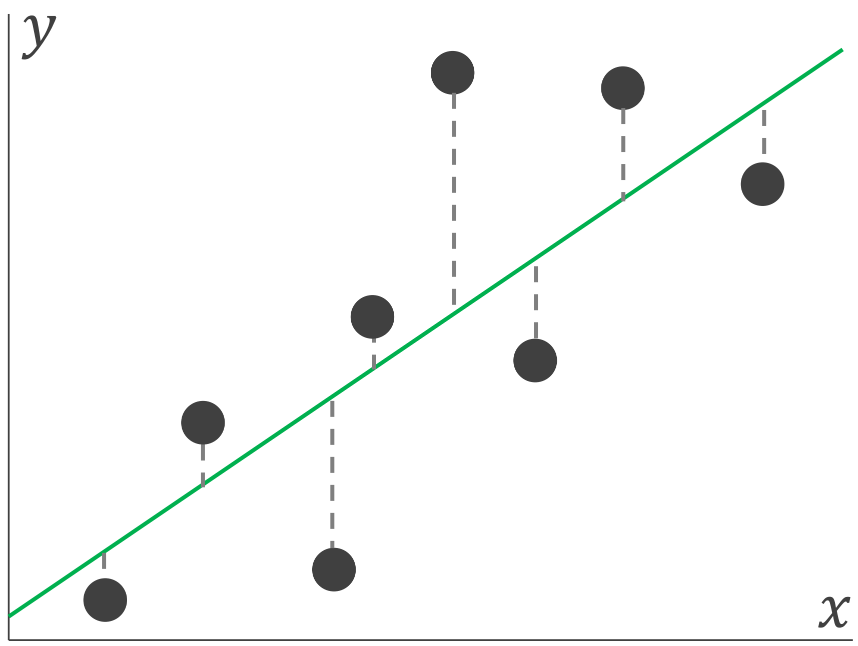


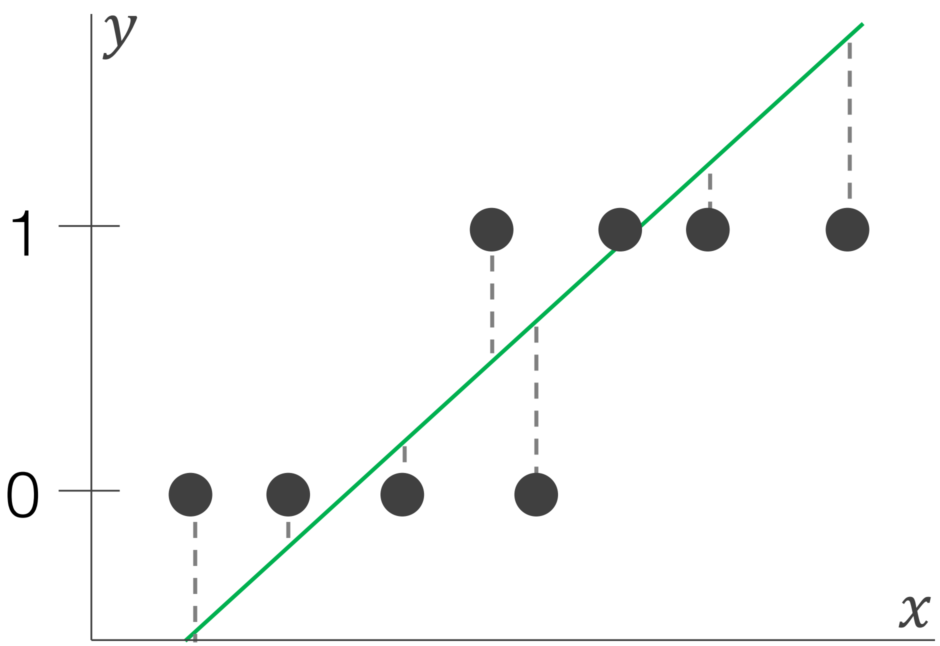
Source: Abu-Mostafa, Learning from Data, Caltech

Linear regression



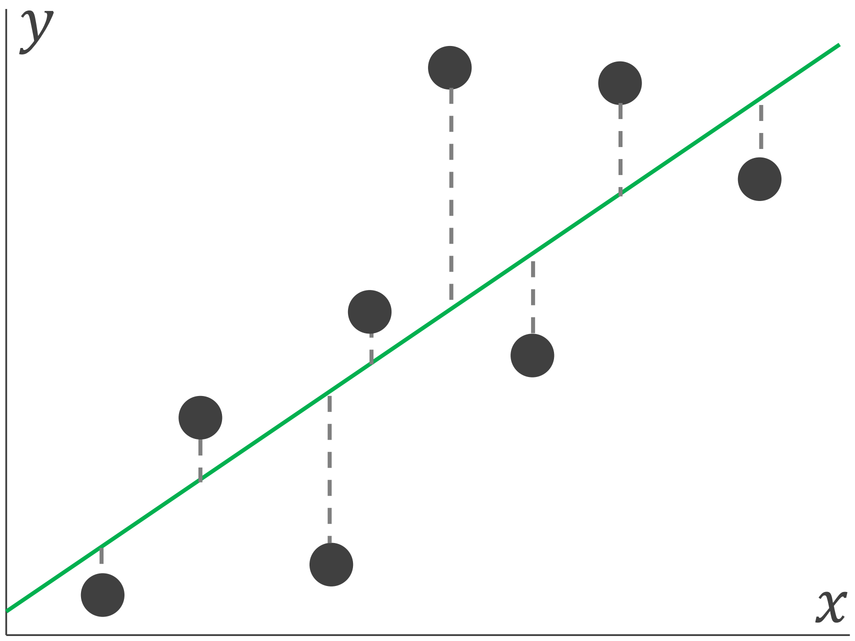
Linear regression

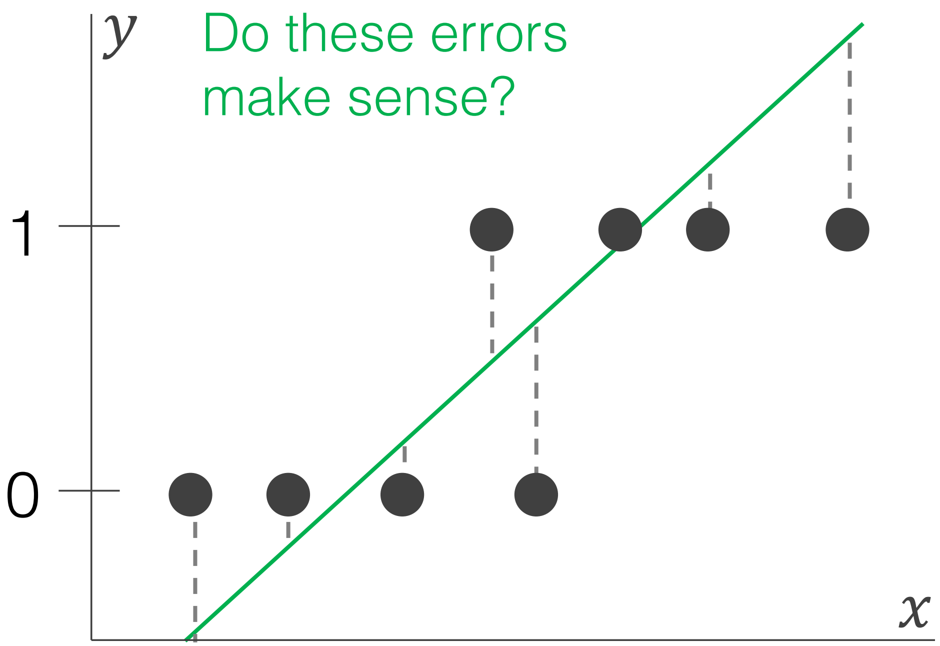




Linear regression applied to a classification problem

Linear regression





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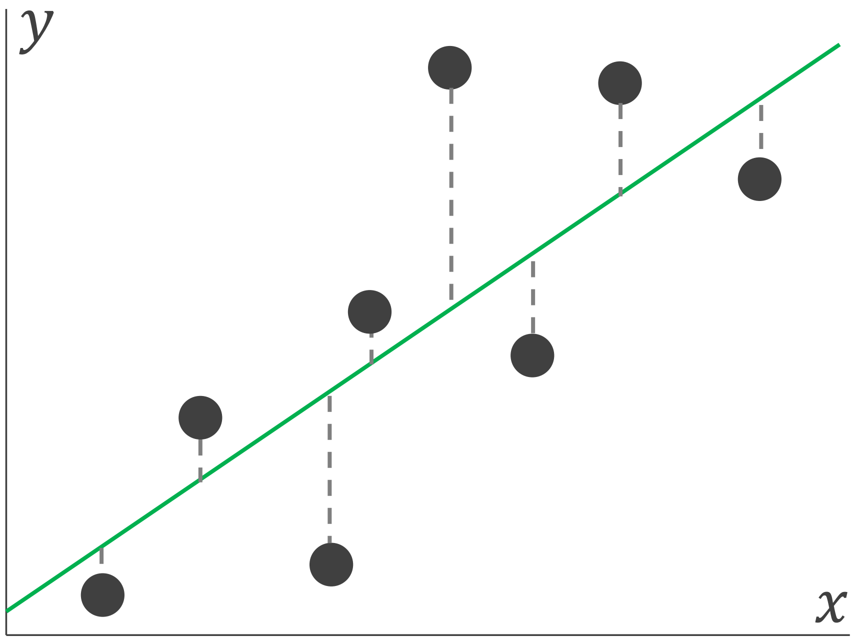
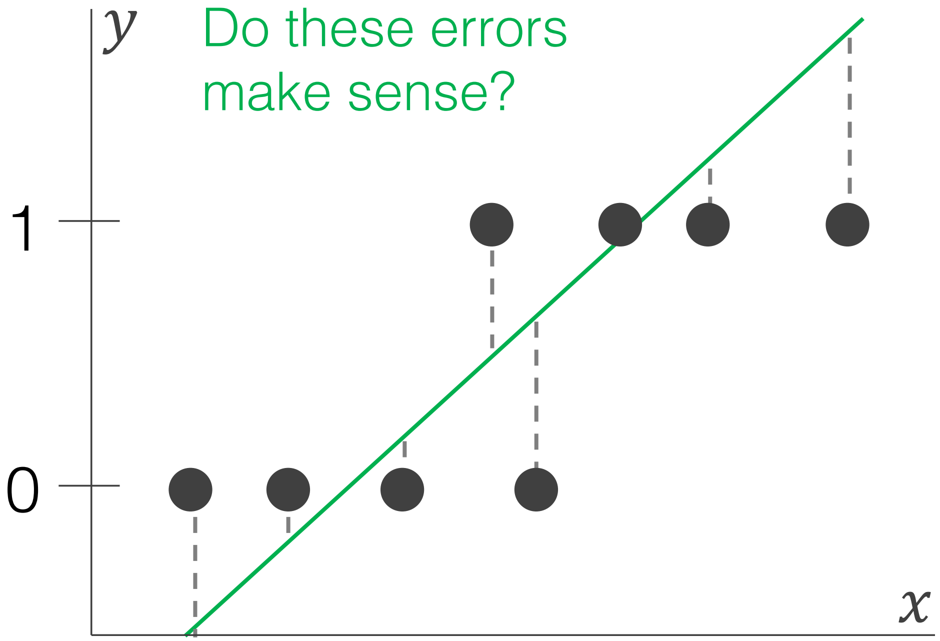
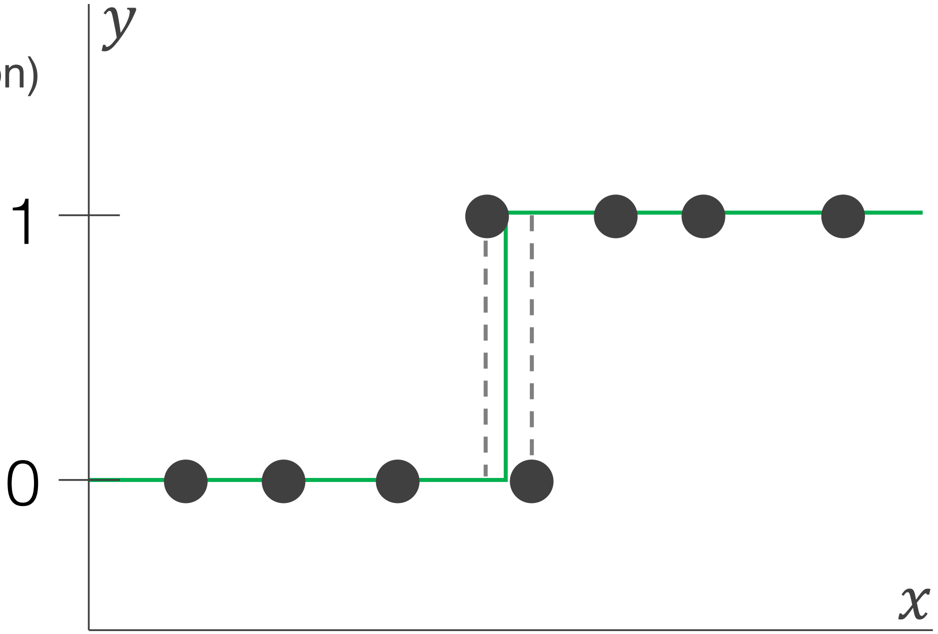




Linear regression applied to a classification problem

Perceptron
(sign activation)



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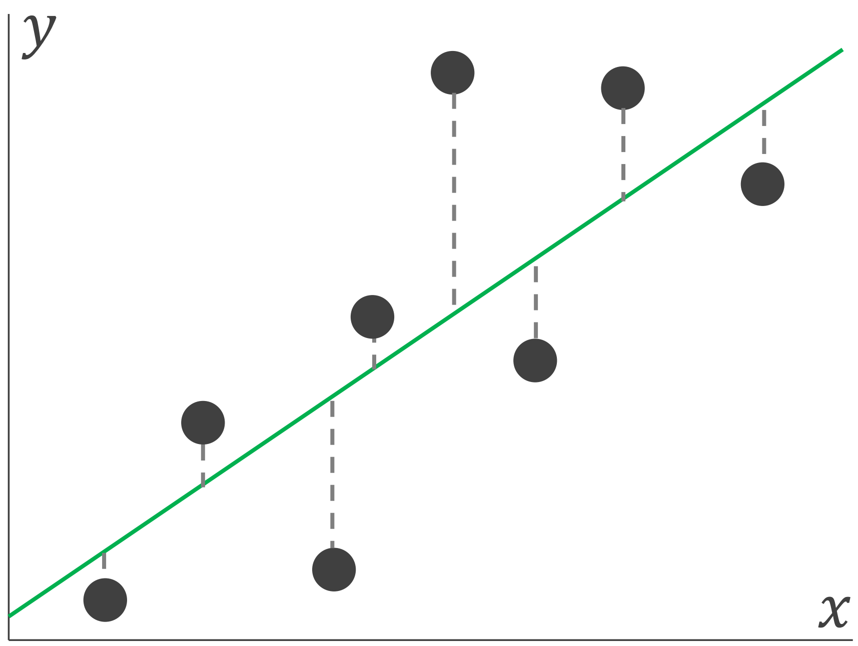

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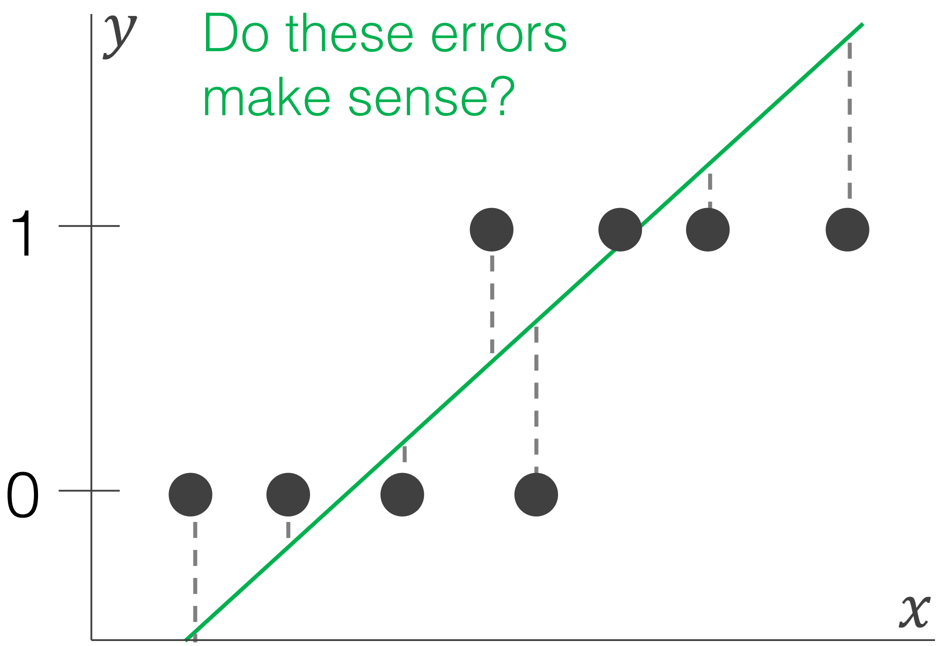
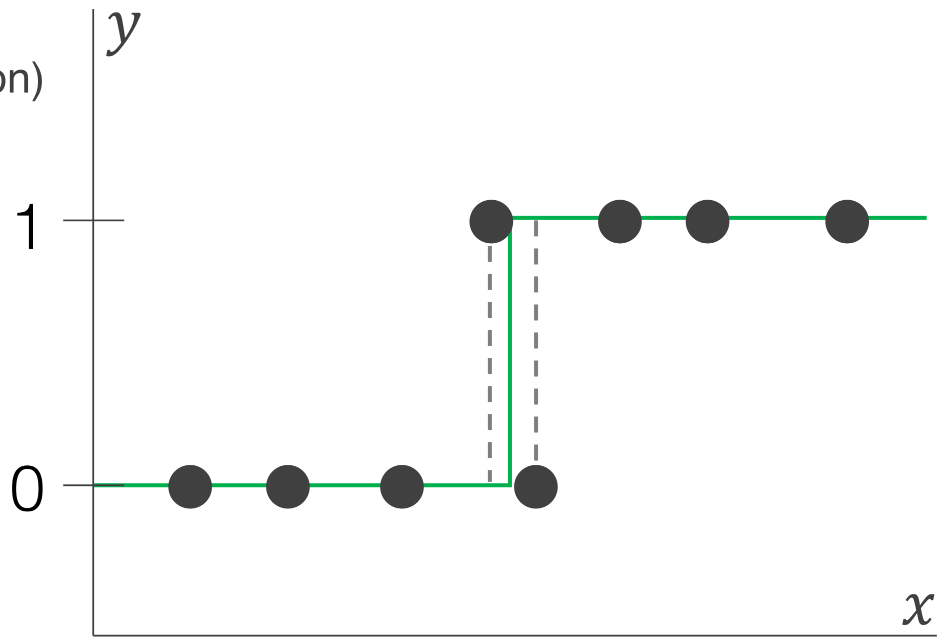
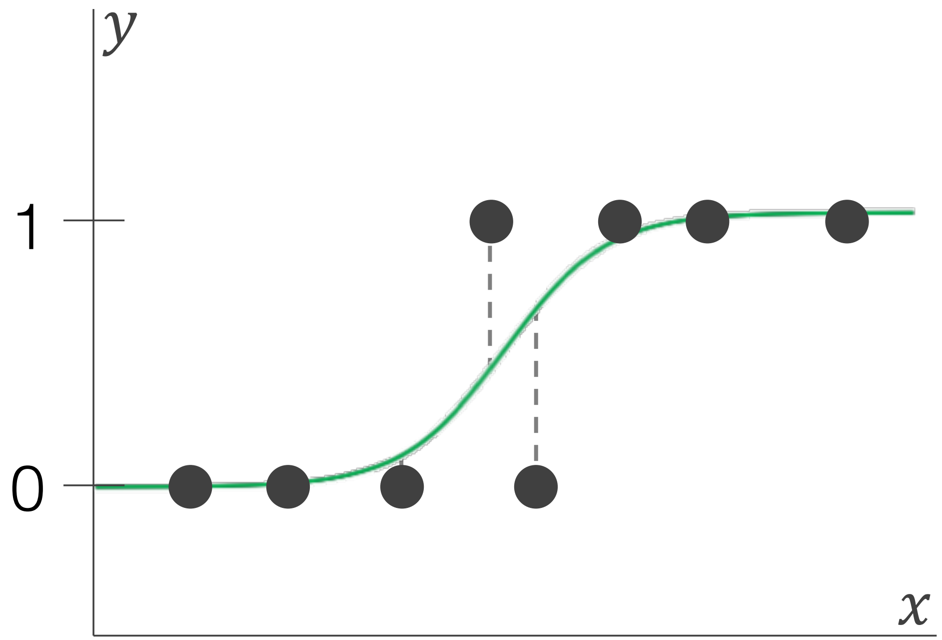


Perceptron (sign activation)



Logistic regression (sigmoid activation)



Perceptron
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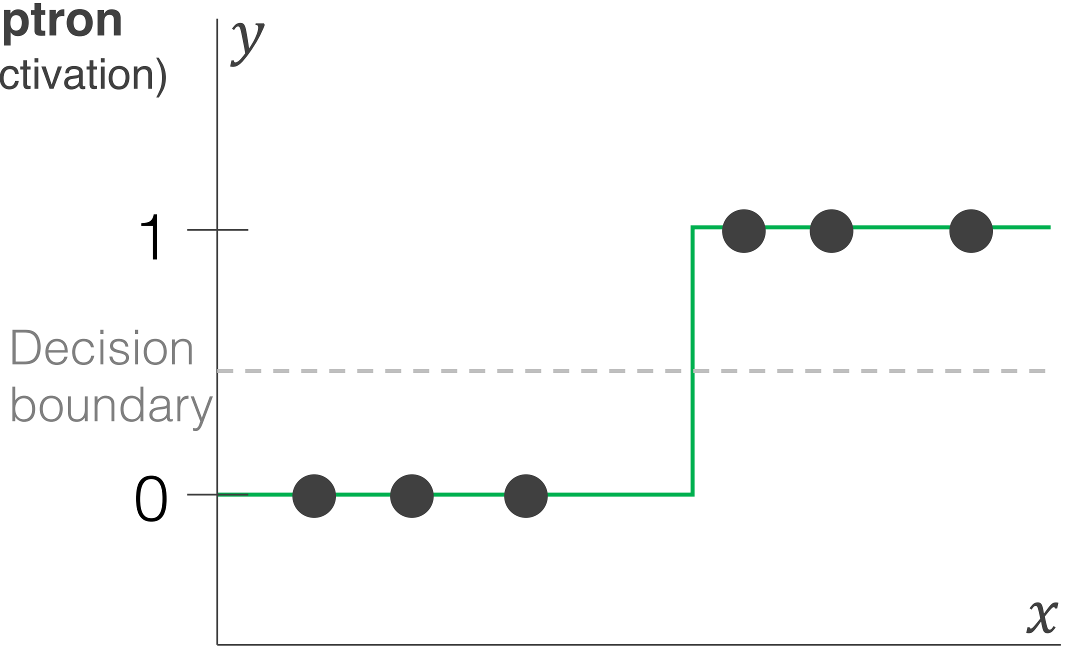
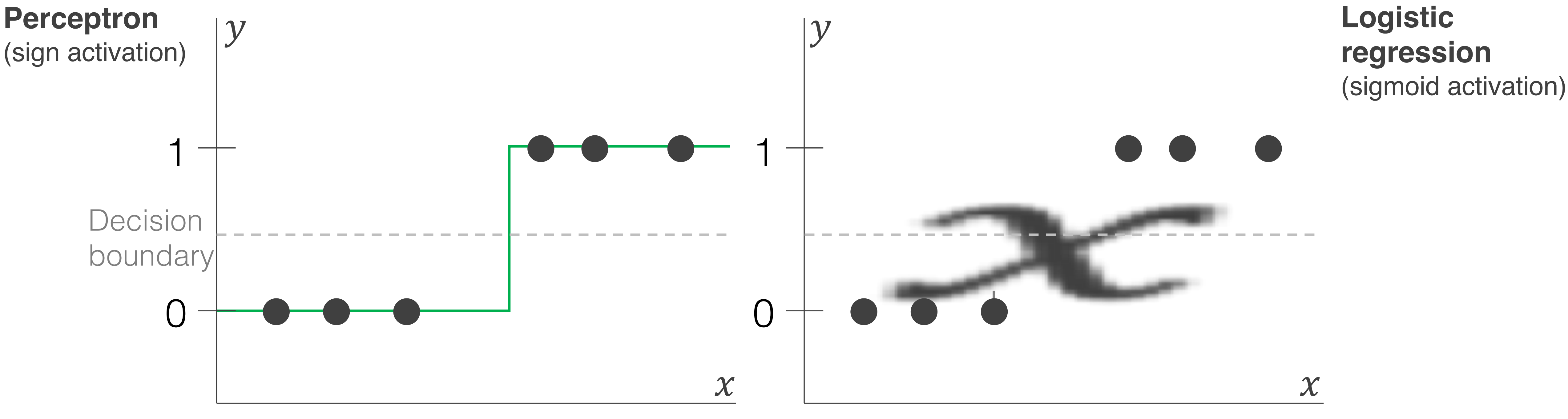
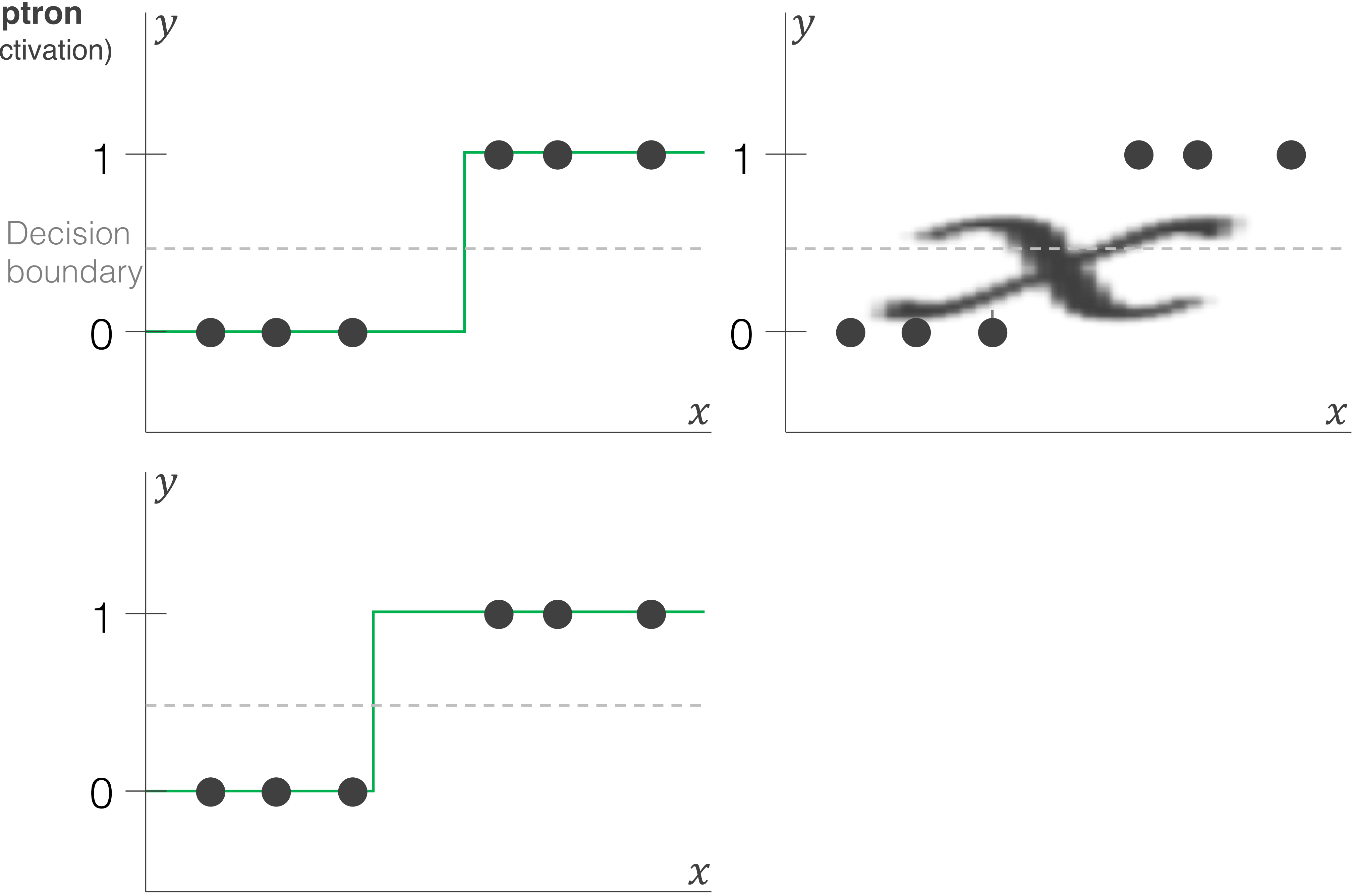
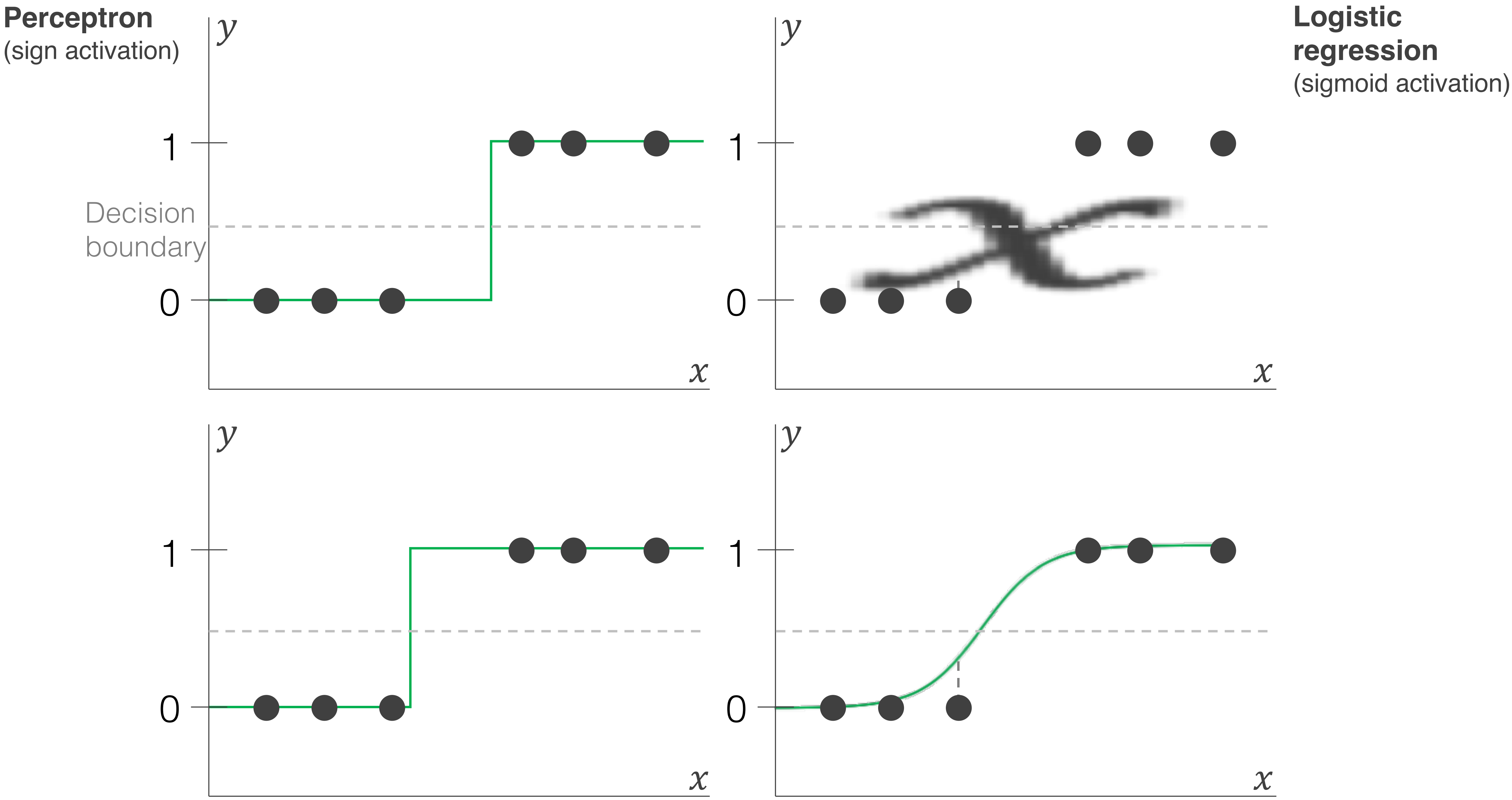



Perceptron
(sign activation)
y
1
Decision
boundary
0
x
Logistic
regression
(sigmoid activation)
y
1
0
x

Perceptron
(sign activation)

Logistic regression
(sigmoid activation)





Perceptron
(sign activation)
Logistic
regression
(sigmoid activation)
y
1
Decision
boundary
0
x
y
1
0
x
y
1
0
x
y
1
0
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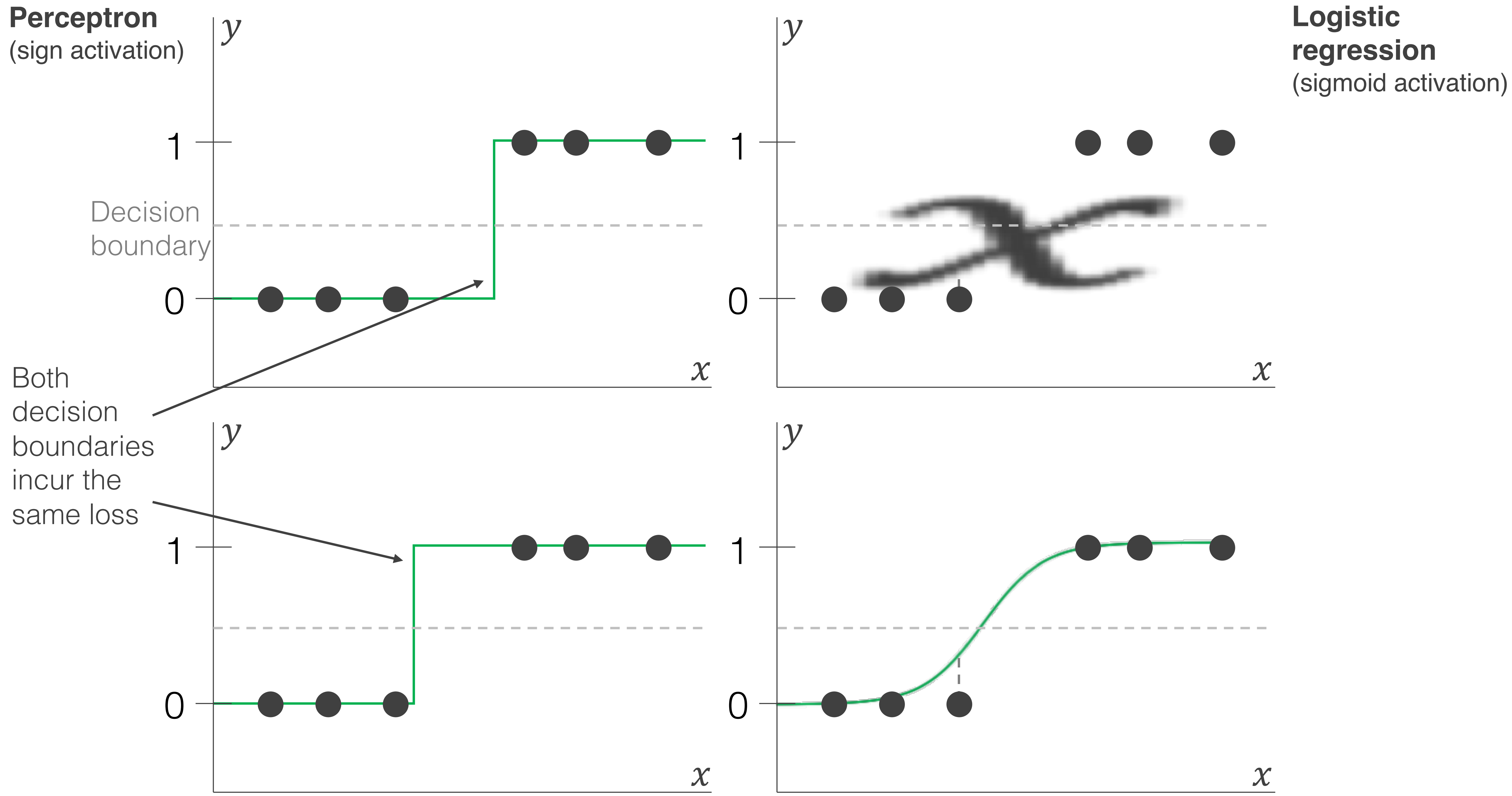
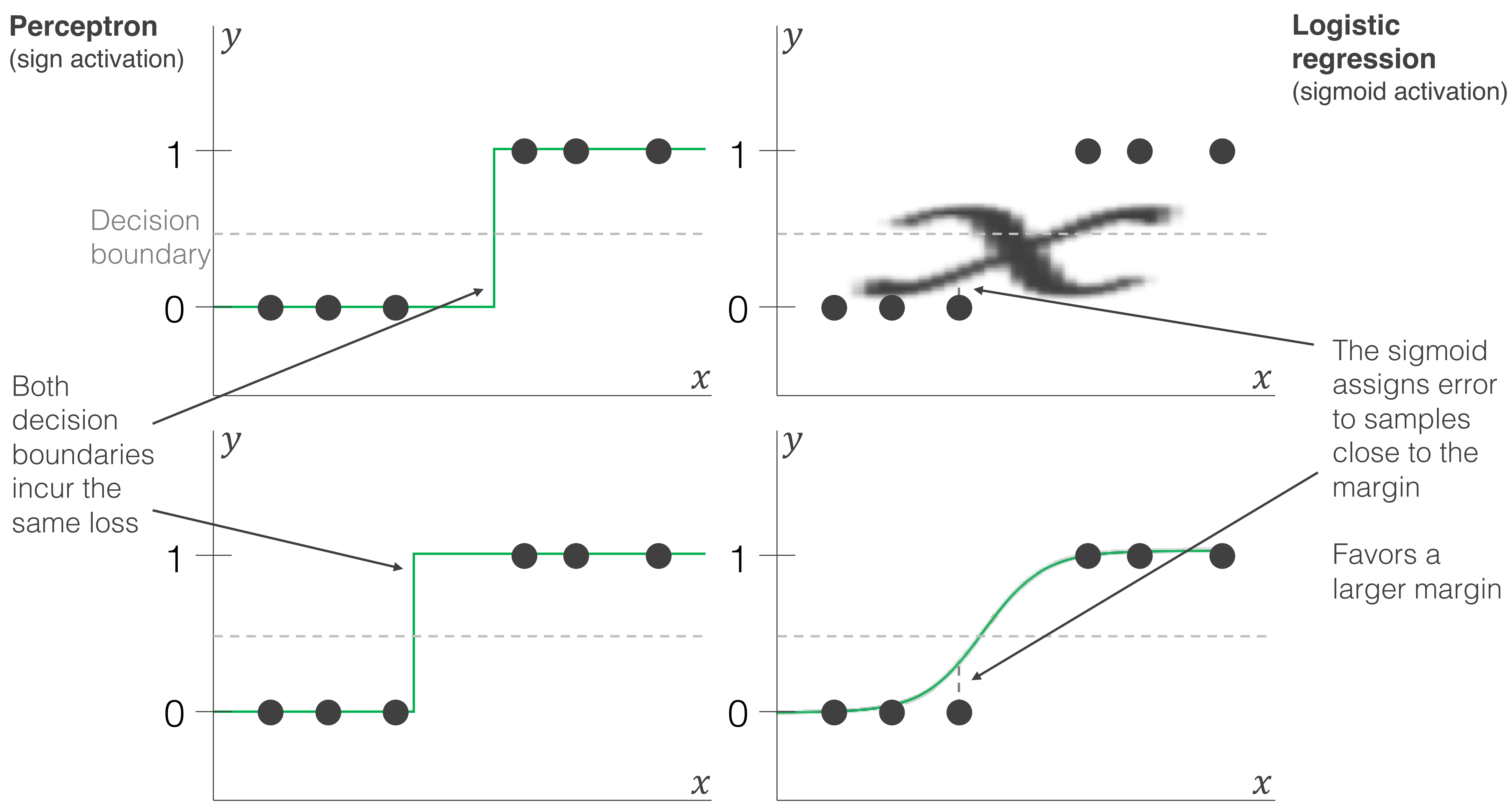

Perceptron
(sign activation)
Logistic regression
(sigmoid activation)
Decision boundary
Both decision boundaries incur the same loss
y
1
0
x


Perceptron
(sign activation)
Logistic regression
(sigmoid activation)
Decision boundary
Both decision boundaries incur the same loss
The sigmoid assigns error to samples close to the margin
Favors a larger margin
y
x
1
0

Sigmoid function

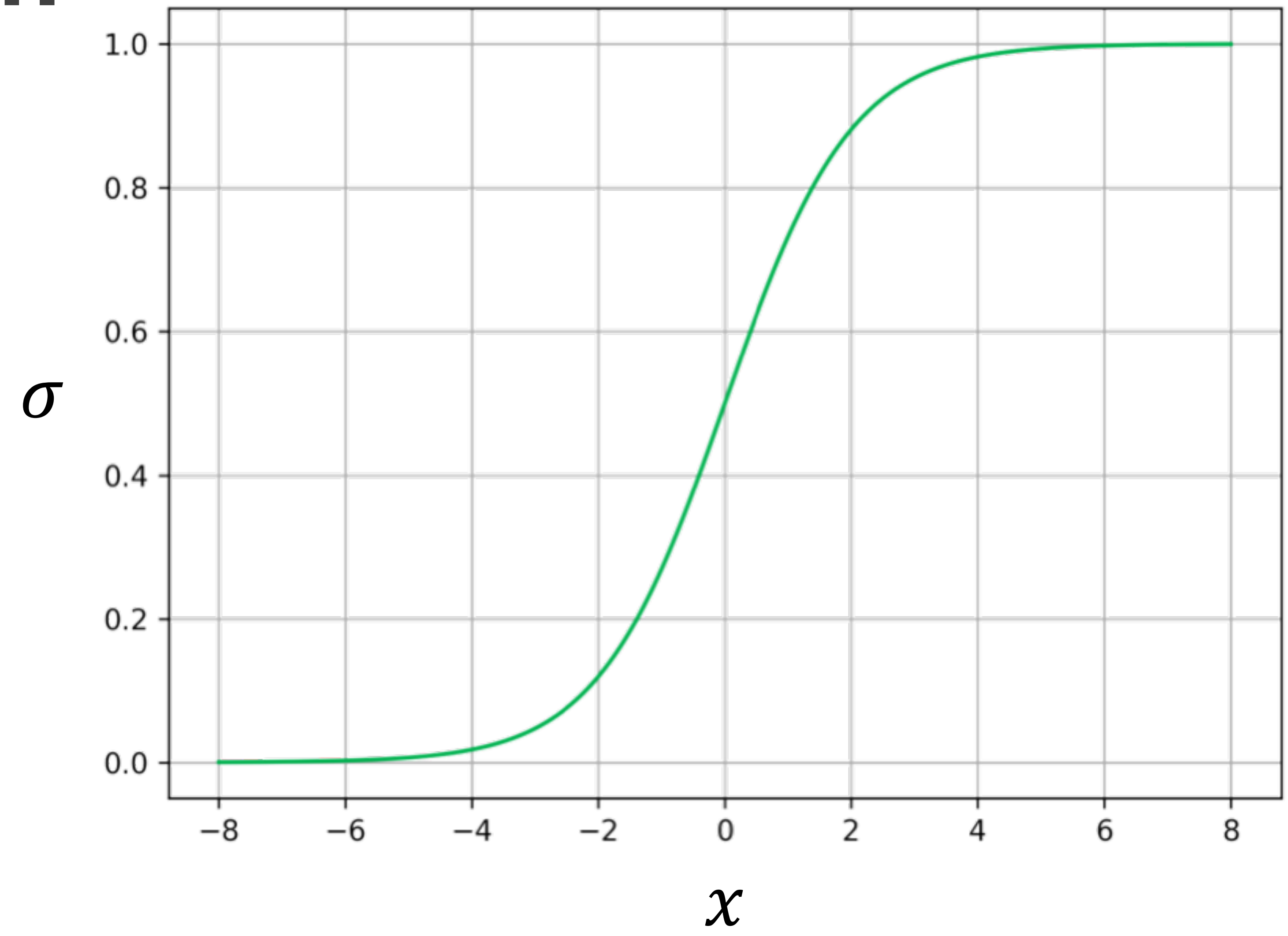
Definition

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

Useful properties

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

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



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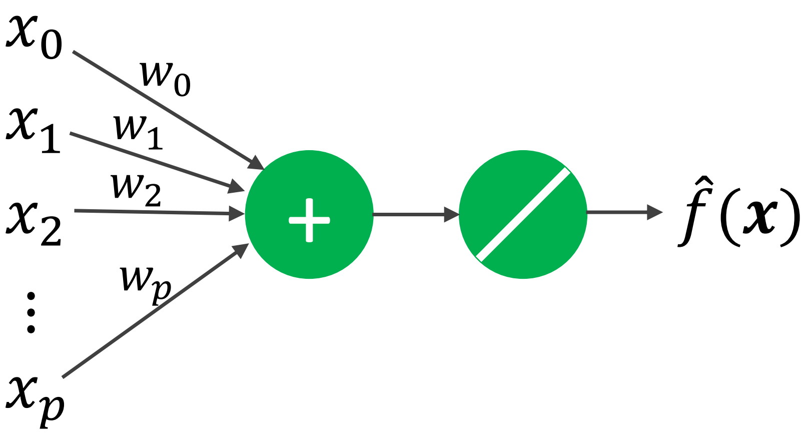
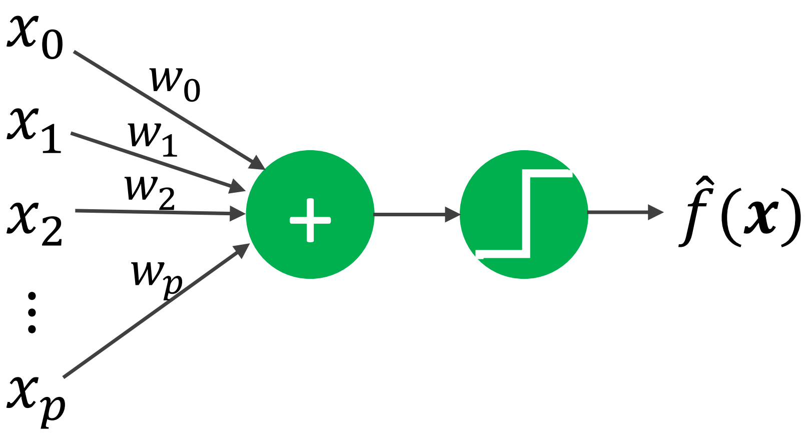


Linear Classification

Perceptron

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

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



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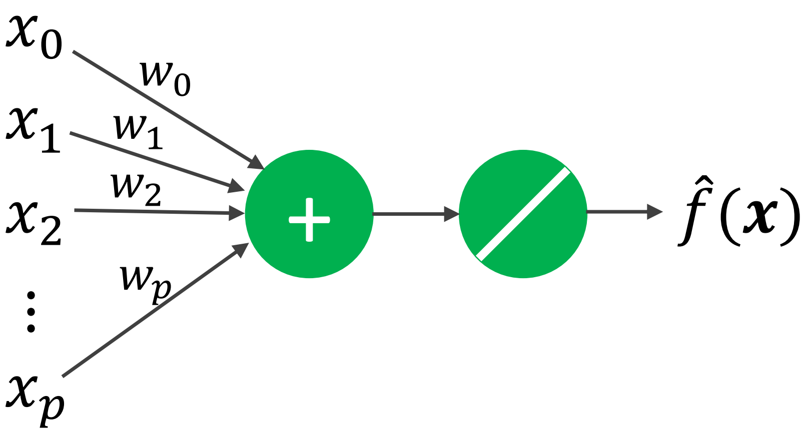

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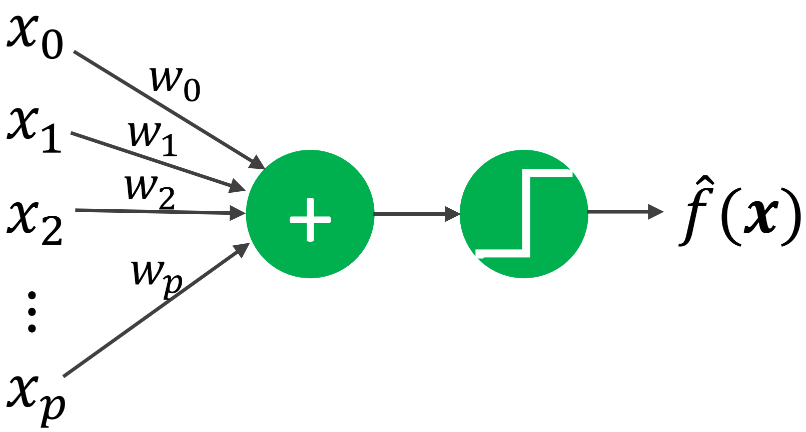

Logistic Regression

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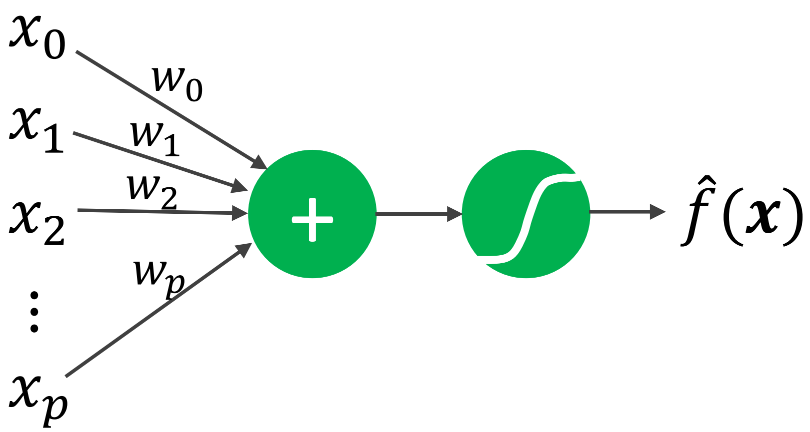
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



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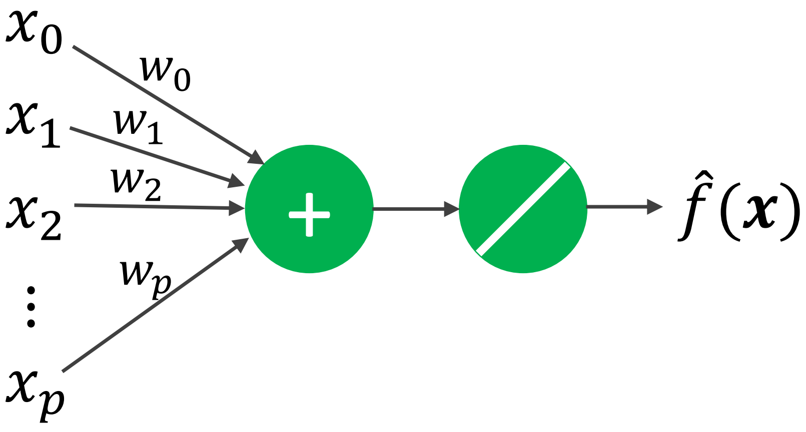

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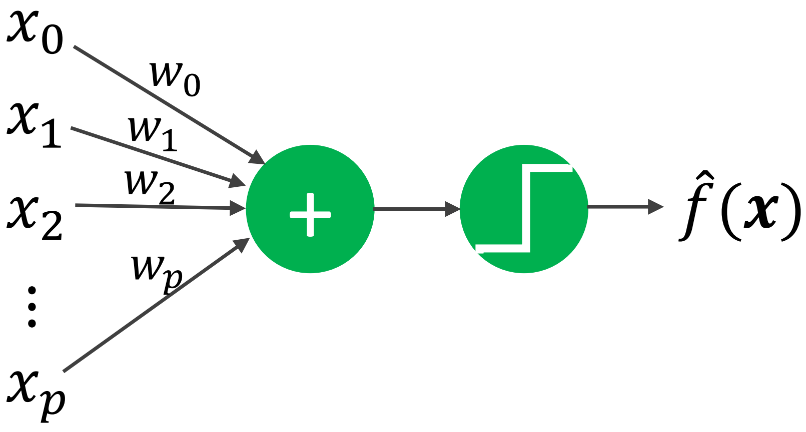

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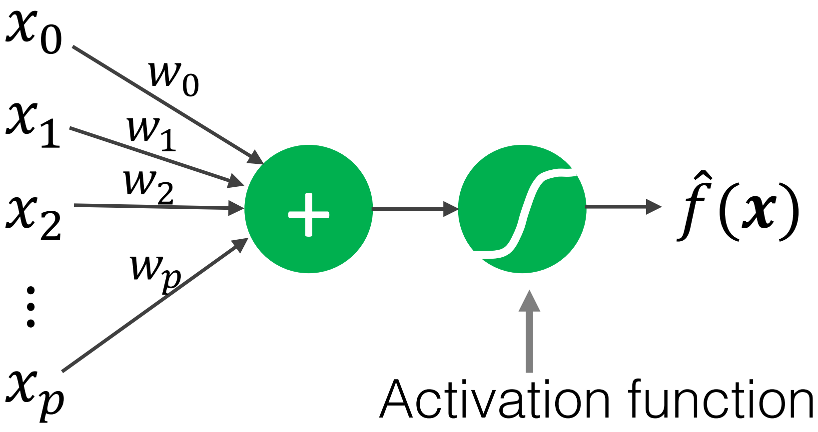

Source: Abu-Mostafa, Learning from Data, Caltech

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

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

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

Plug in our model

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

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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

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

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

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

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

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The interpretation of the Likelihood

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

Source: Malik Magdon-Ismail, Learning from Data

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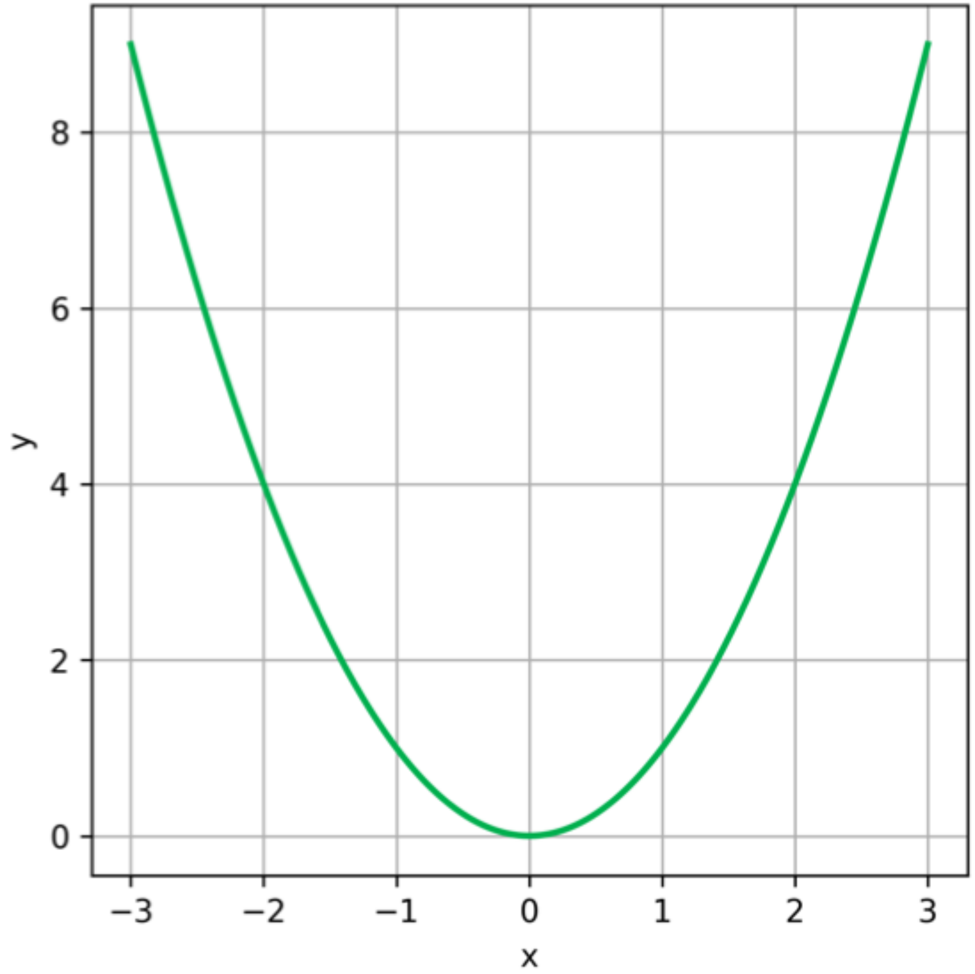
This is not solvable in closed form: need a new approach

Gradient descent

Minimize $y = x^2$



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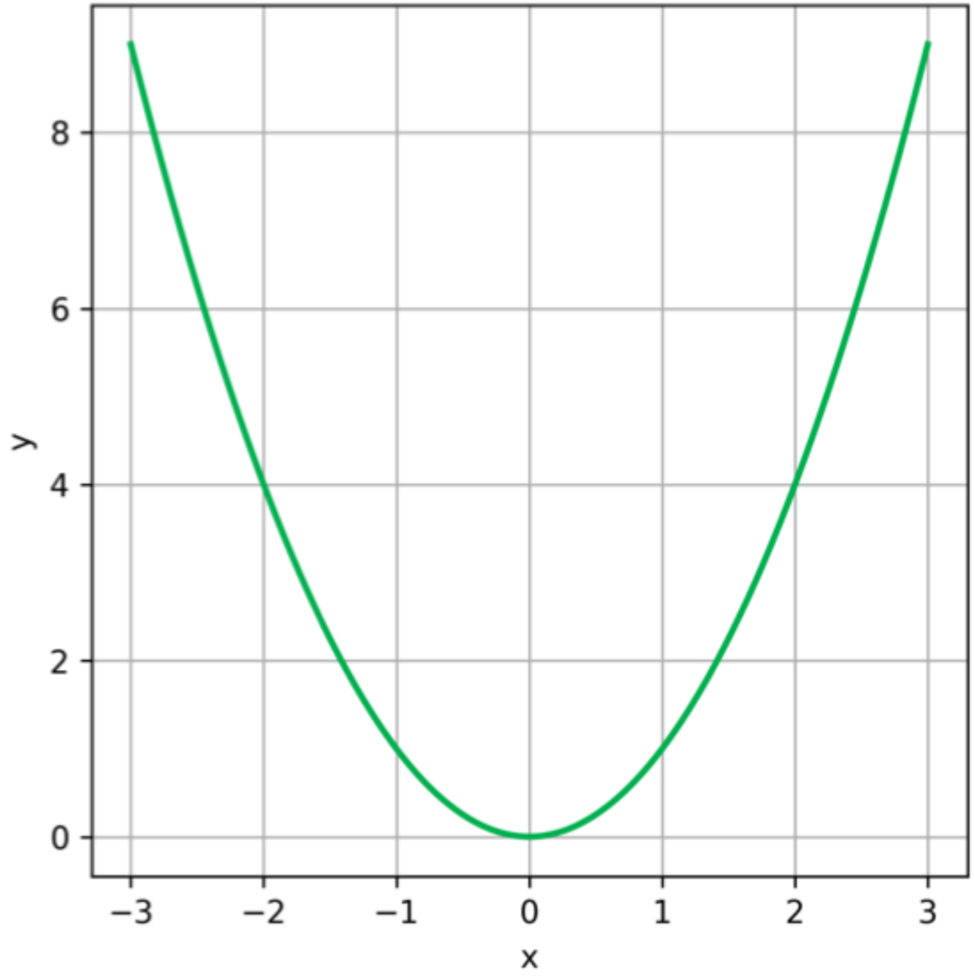

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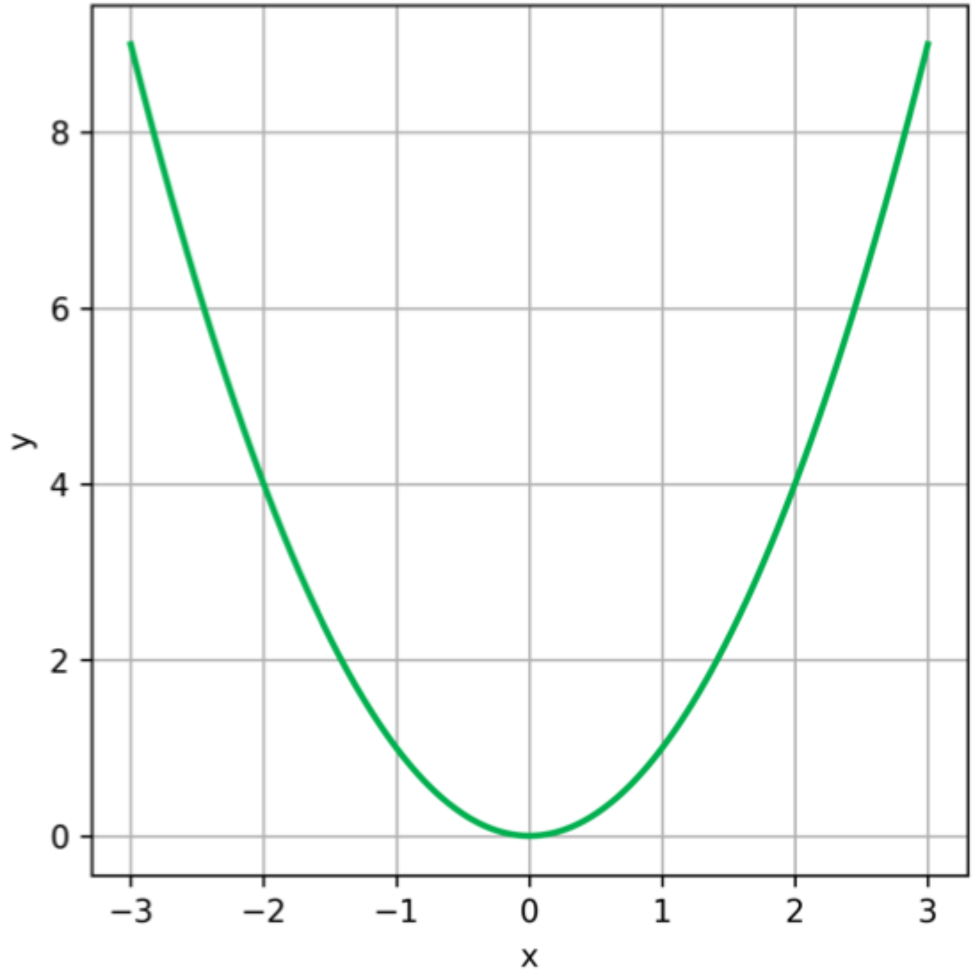
$$\boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} + \eta \boldsymbol{v}$$

Learning rate

Direction to move in



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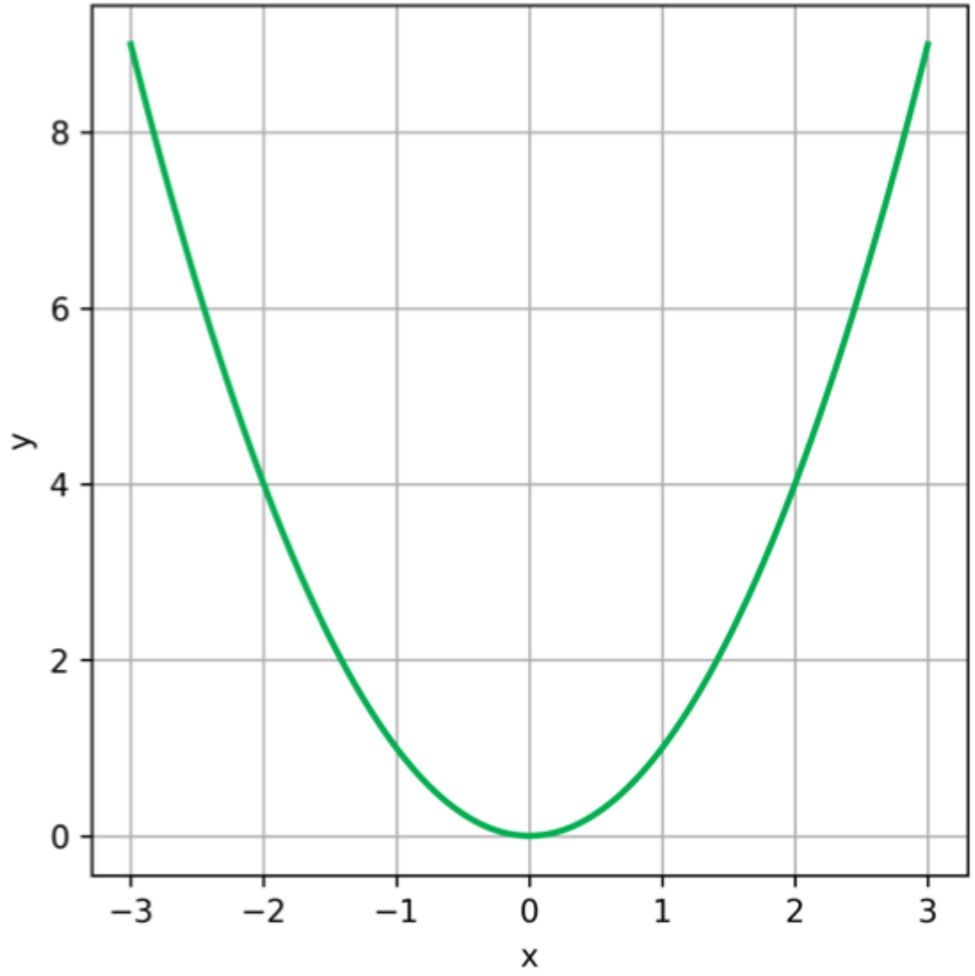
Minimize $f(x) = x^2$



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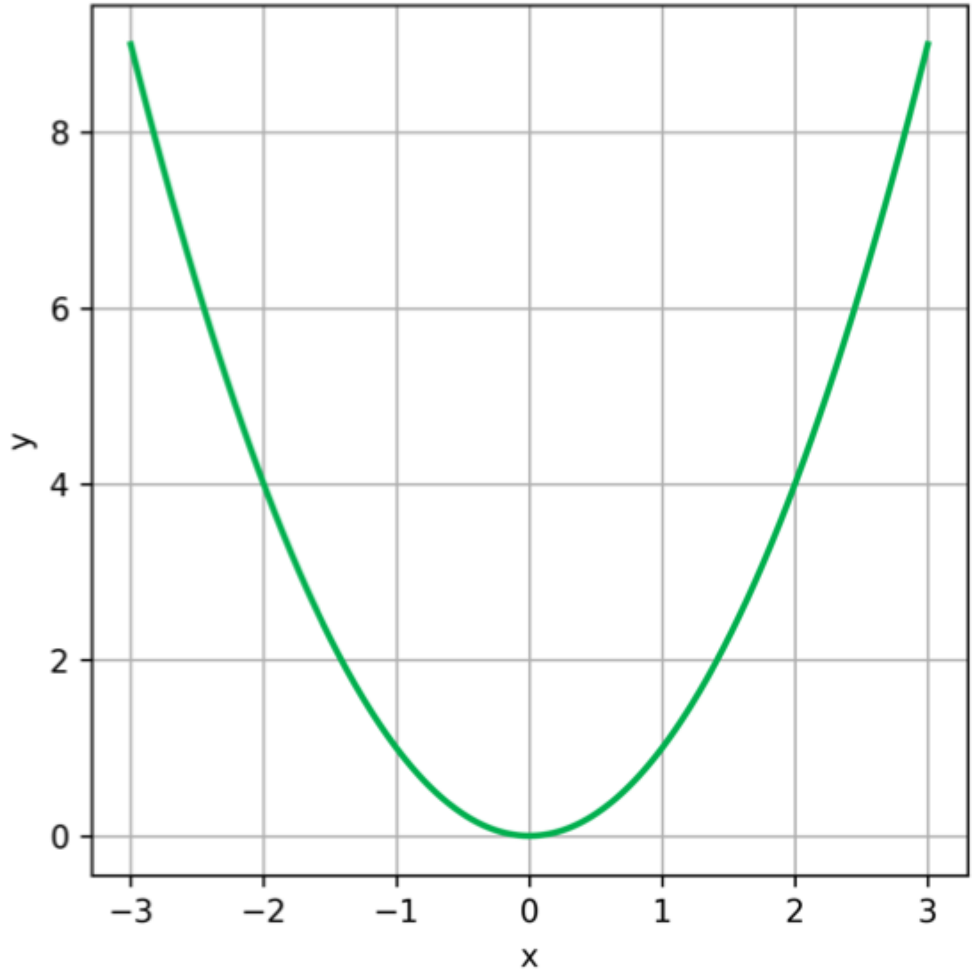
The gradient points in the direction of steepest **positive** change



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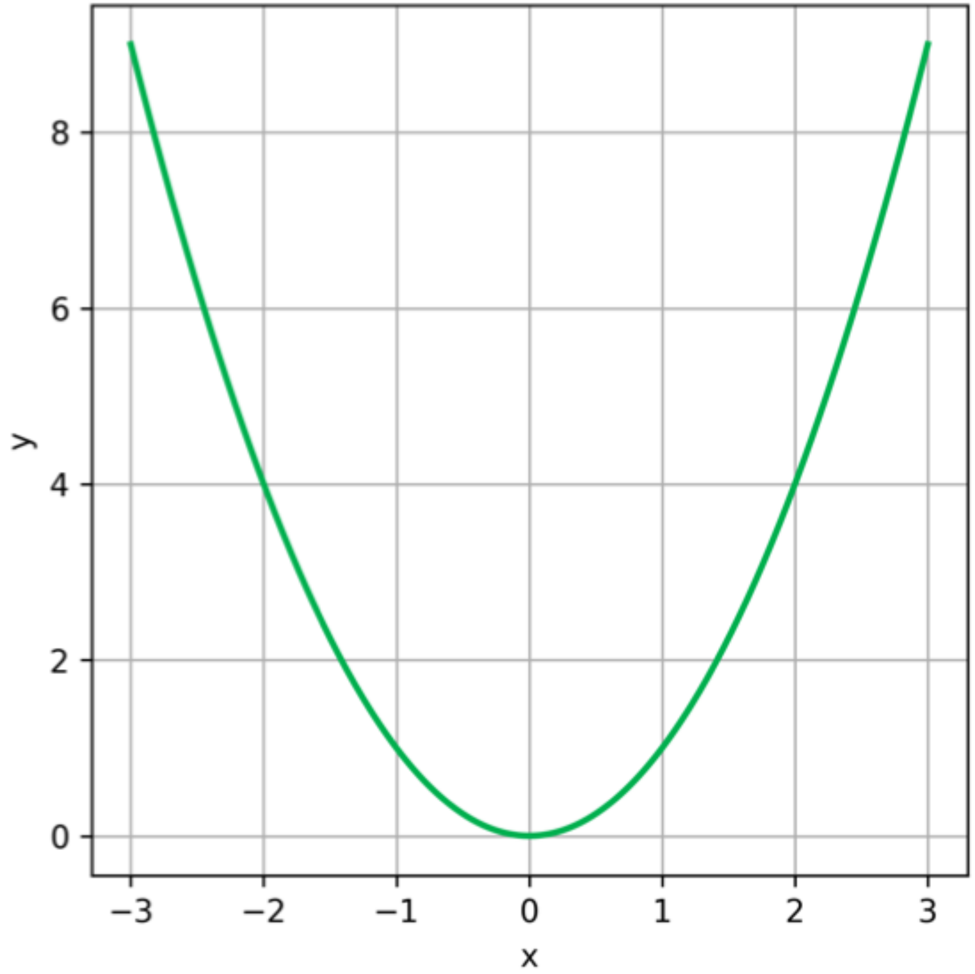

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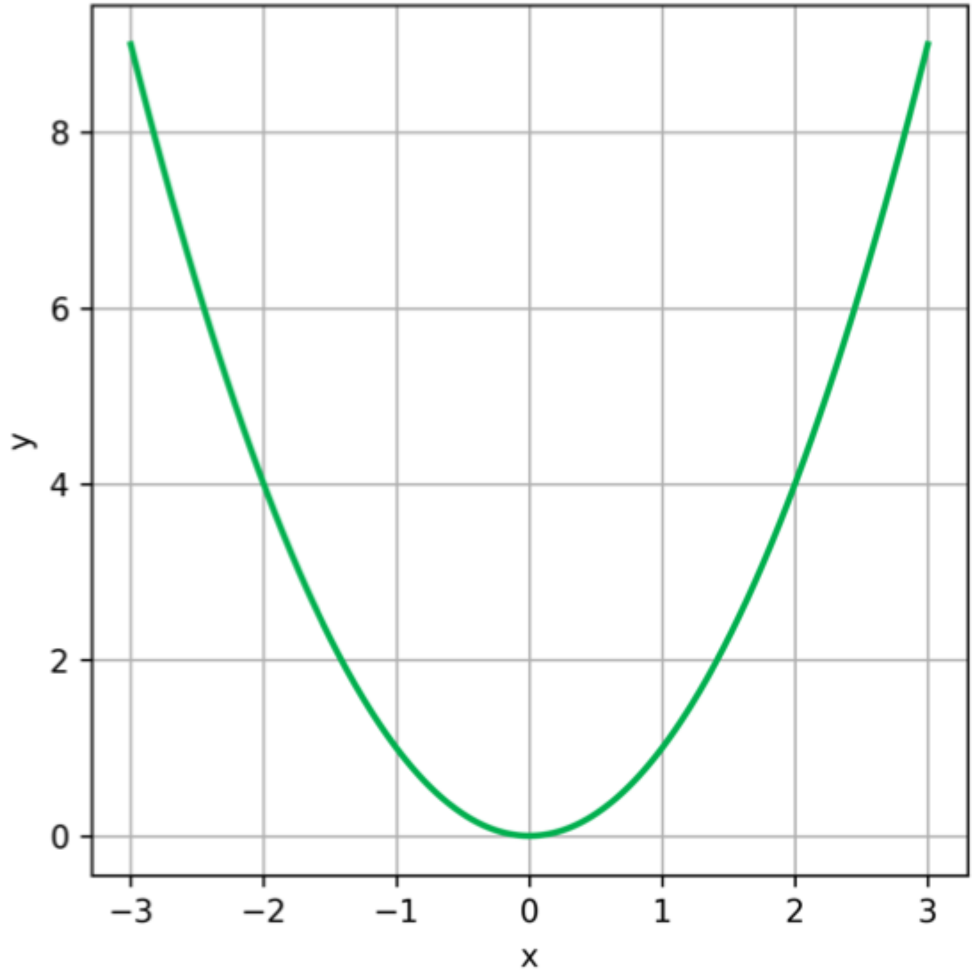

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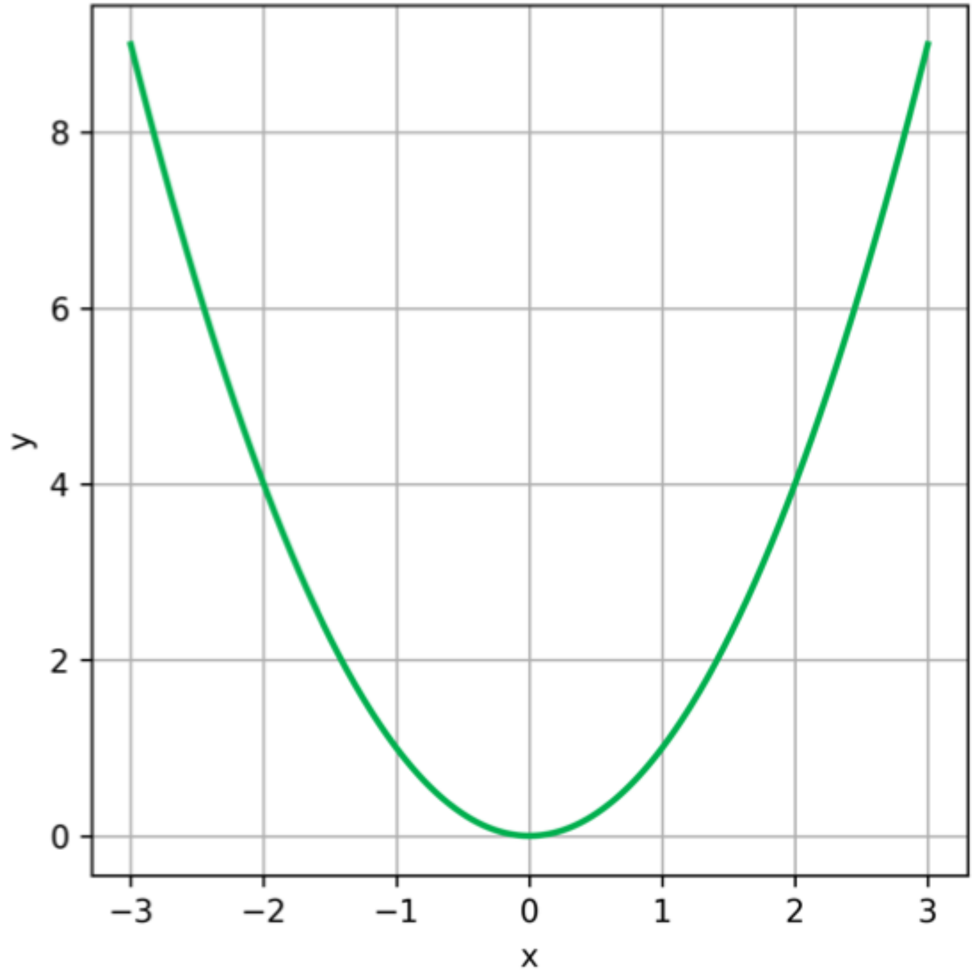

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$$\boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} - (0.25)(2\boldsymbol{x}^{(i)})$$

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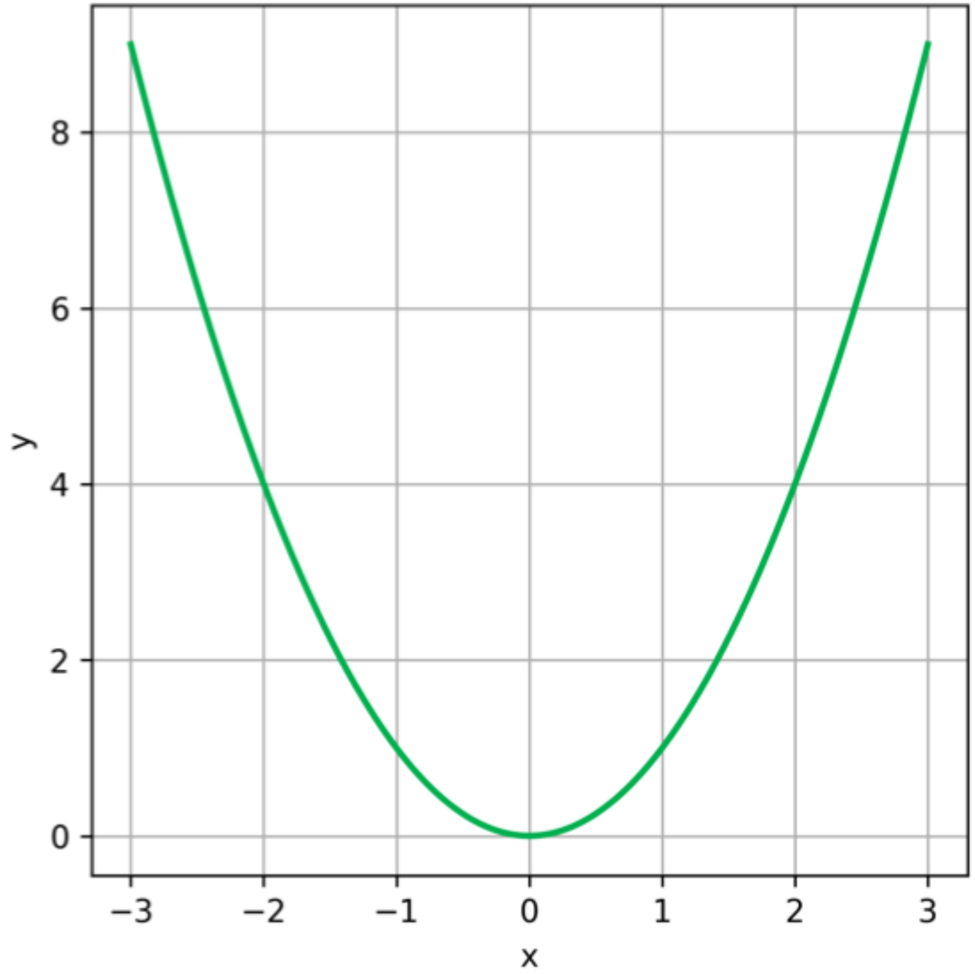

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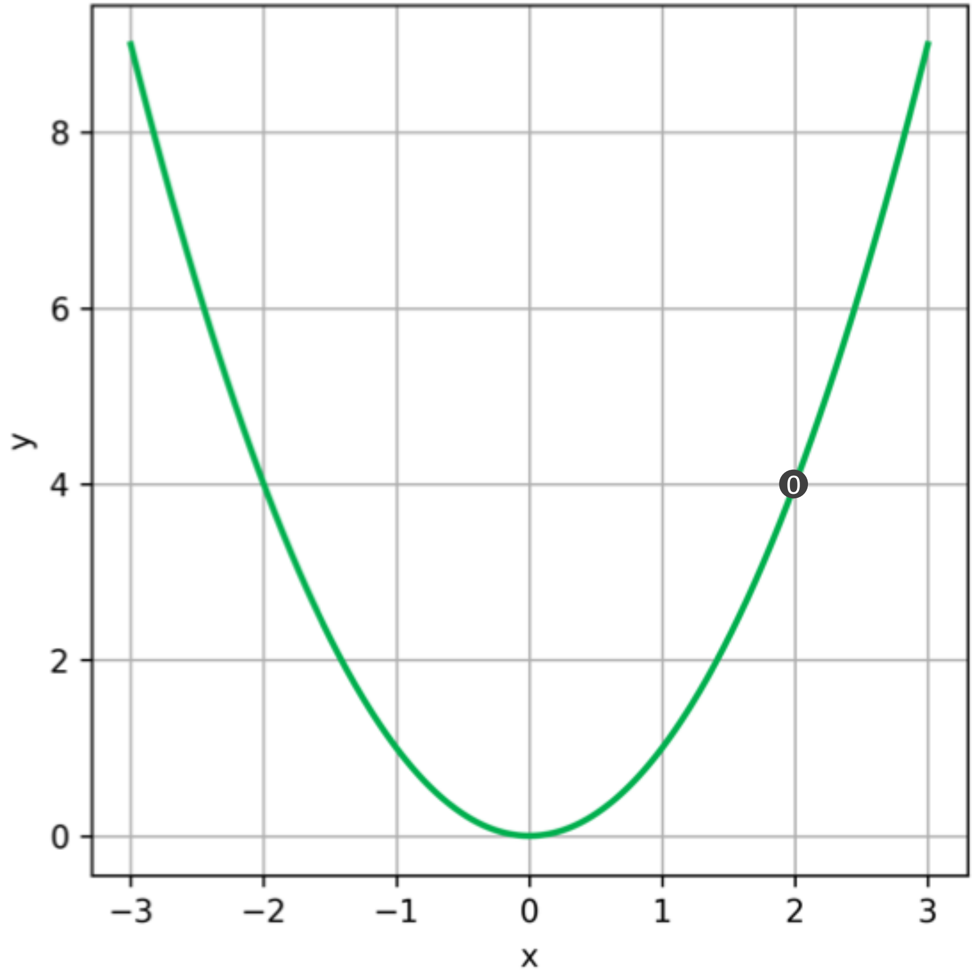
i	$x^{(i)}$	$y^{(i)}$
0	2	4



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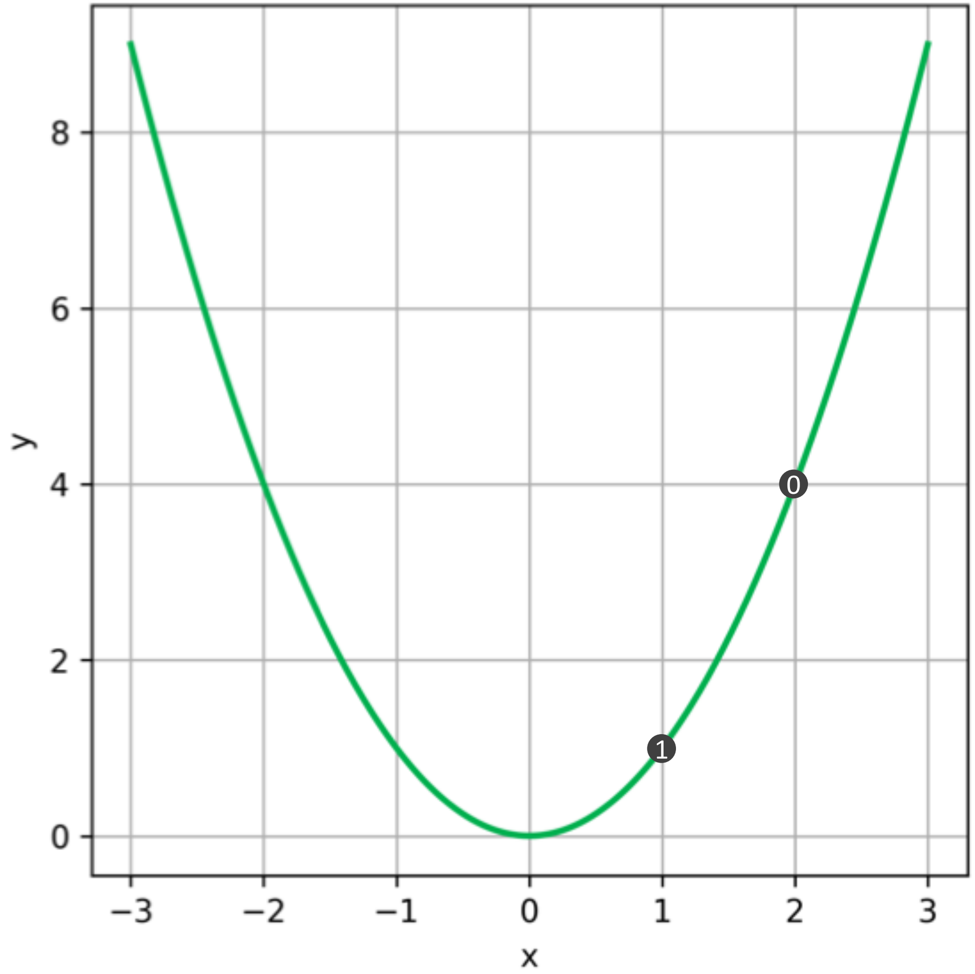
1	1	1



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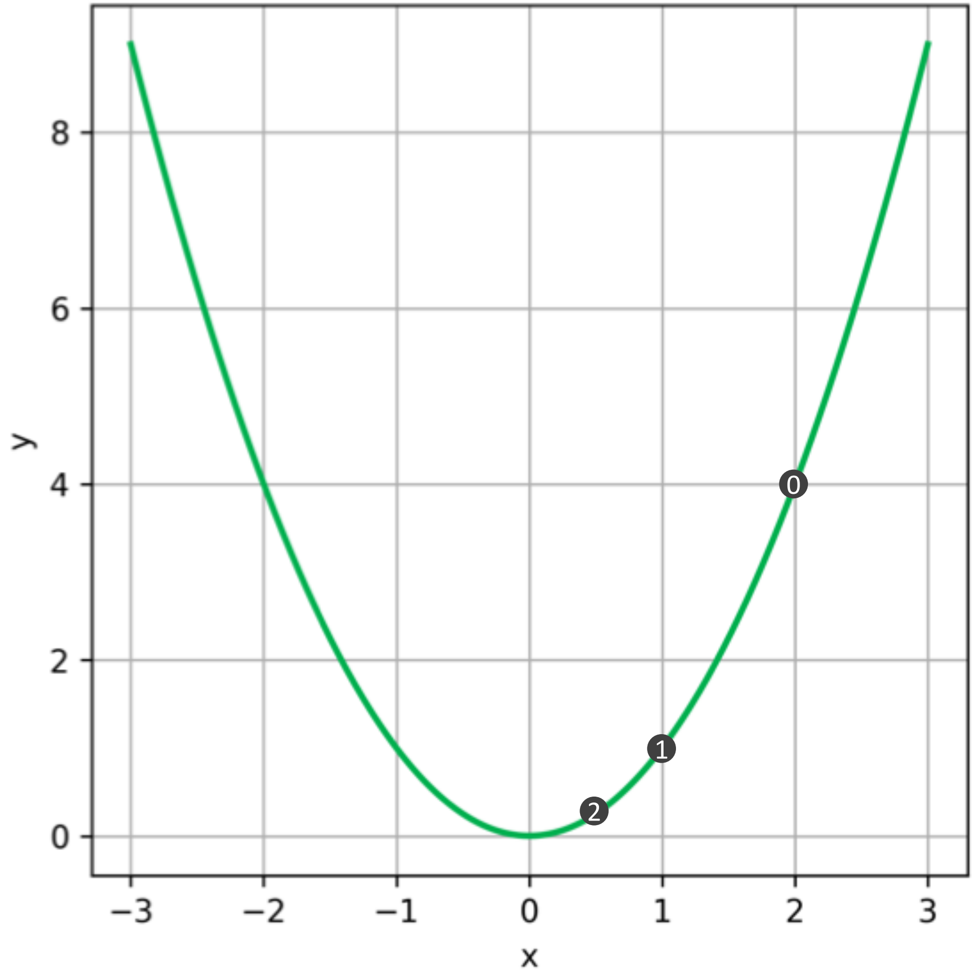

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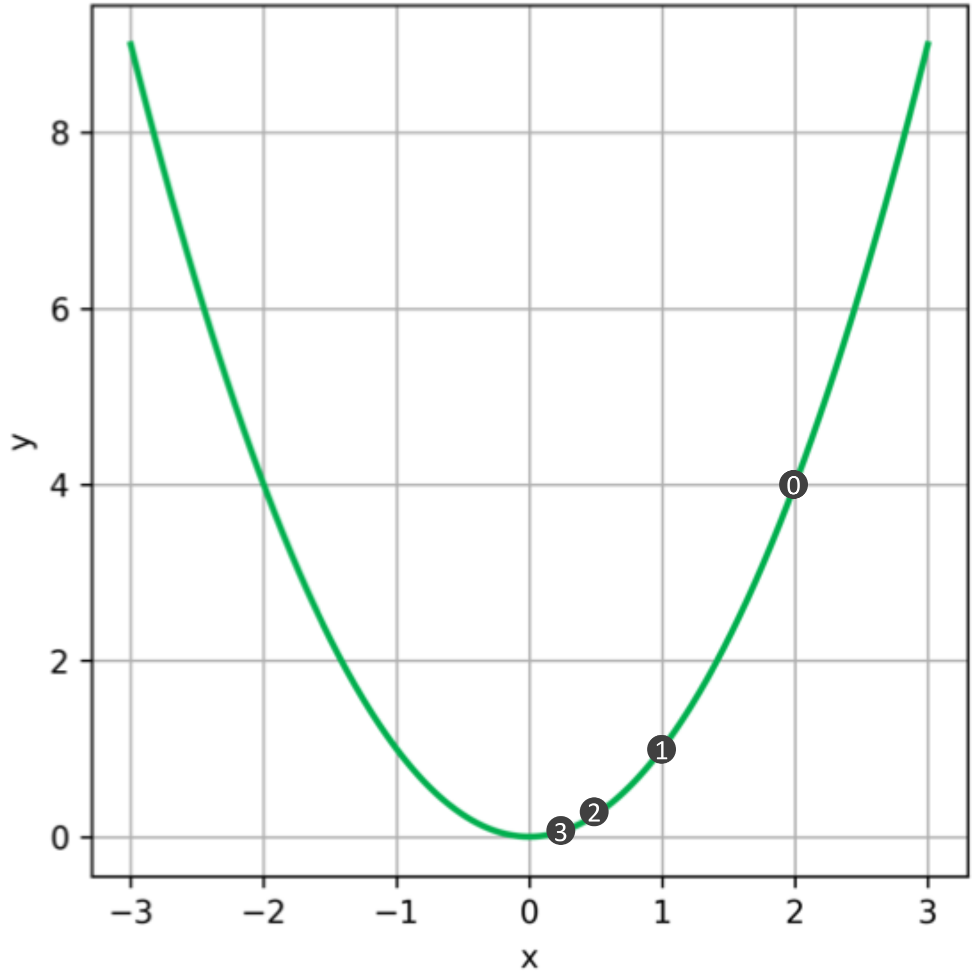

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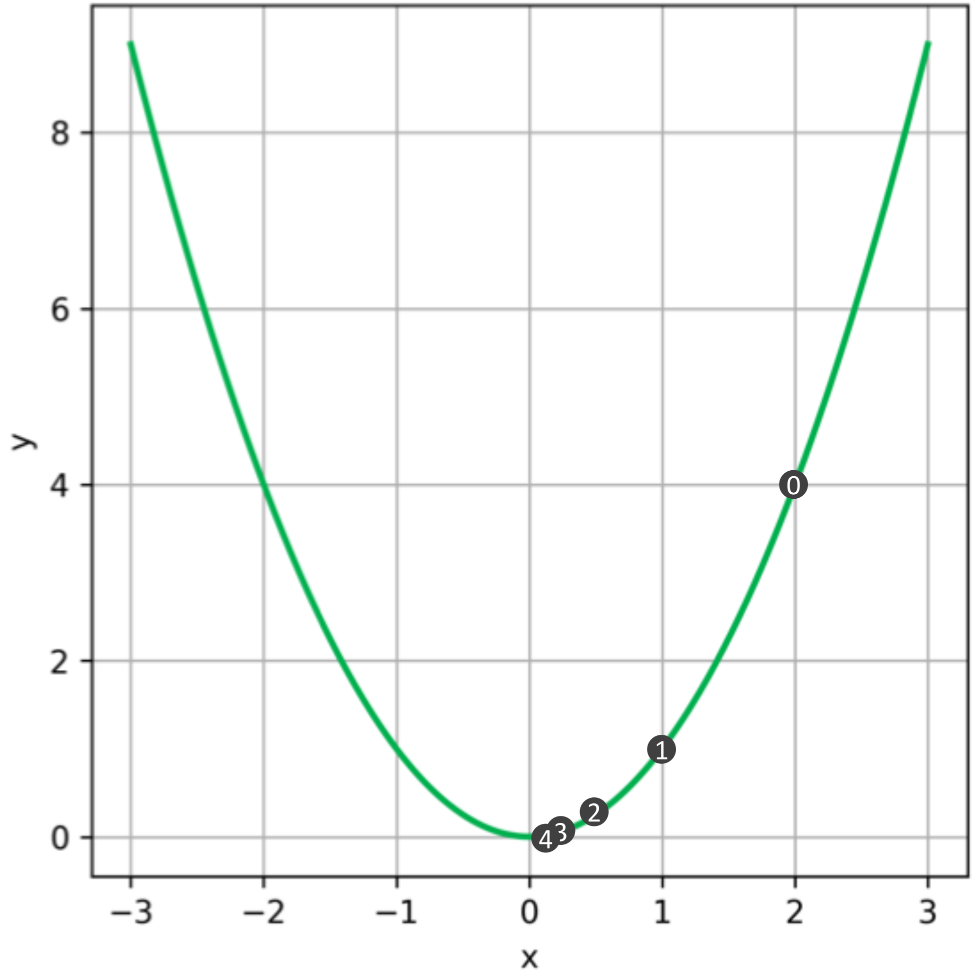
0	2	4
1	1	1
2	0.5	0.25
3	0.25	0.0625
4	0.125	0.0156



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