Daily Inspiration

Today

- Recap yesterday
- Logistic regression: using regression tools for classification
- Neural network basics

Yesterday

- Cost function: (differentiable) function that shows how wrong an estimate is for given parameters.
- Gradient descent: one common way to minimise the cost function automatically, i.e. to get optimal parameters
- Linear regression: very simple model that assumes that value to predict is linear combination of input features.
- Overfitting and underfitting, bias and variance: want our model to work wel for unseen data. Need just enough model freedom given the complexity of our problem. How:
  - Cross-validation to measure ability to generalise + get best hyperparameters
  - Use learning curves to diagnose bias vs. variance

Gradient descent in linear algebra

- Goal gradient descent: take a small step in every parameter such that you get closer to the minimum of the cost. Return new theta's.

$$\theta_{0new} = \theta_0 - \frac{a}{m} \sum_{i=1}^{m} ((h_\theta(x^{(i)}) - y^{(i)}) \cdot 1)$$

$$\theta_{1new} = \theta_1 - \frac{a}{m} \sum_{i=1}^{m} ((h_\theta(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)})$$

$$\theta_{2new} = \theta_2 - \frac{a}{m} \sum_{i=1}^{m} ((h_\theta(x^{(i)}) - y^{(i)}) \cdot x_2^{(i)})$$

Gradient descent in linear algebra

We have data, known values, and initial theta's:

$$X = \begin{bmatrix} 1 & feat_1 val_1 & feat_2 val_1 \\ 1 & feat_1 val_2 & feat_2 val_2 \end{bmatrix}; y = \begin{bmatrix} 10.23 \\ -4 \end{bmatrix}; params = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$$

Get predicted values:

$$\begin{bmatrix} 1 & feat_1 val_1 & feat_2 val_1 \\ 1 & feat_1 val_2 & feat_2 val_2 \end{bmatrix} @ \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} 9.23 \\ -2.5 \end{bmatrix}$$

2 by 3 times 3 by 1 gives 2 by 1 (rows by columns)

Get errors:

$$errs = \begin{bmatrix} 9.23 \\ -2.5 \end{bmatrix} - y = \begin{bmatrix} 9.23 \\ -2.5 \end{bmatrix} - \begin{bmatrix} 10.23 \\ -4 \end{bmatrix} = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}$$

Gradient descent in linear algebra

$$errs = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}$$

$$\theta_{0new} = \theta_0 - \frac{a}{m} \sum_{i=1}^{m} \left(\boxed{\left(h_\theta(x^{(i)}) - y^{(i)} \right)} \cdot 1 \right)$$

$$\theta_{1new} = \theta_1 - \frac{a}{m} \sum_{i=1}^{m} \left(\boxed{\left(h_\theta(x^{(i)}) - y^{(i)} \right)} \cdot x_1^{(i)} \right)$$

$$\theta_{2new} = \theta_2 - \frac{a}{m} \sum_{i=1}^{m} \left(\boxed{\left(h_\theta(x^{(i)}) - y^{(i)} \right)} \cdot x_2^{(i)} \right)$$

Gradient descent in linear algebra

Calculate, for each feature, sum of each error times that feature:

$$\begin{bmatrix} -1 \\ 1.5 \end{bmatrix}^T = \begin{bmatrix} -1 & 1.5 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 1.5 \end{bmatrix} @ \begin{bmatrix} 1 & feat_1 val_1 & feat_2 val_1 \\ 1 & feat_1 val_2 & feat_2 val_2 \end{bmatrix} =$$

$$\begin{bmatrix} -1 \cdot 1 + 1.5 \cdot 1 & -1 \cdot feat_1 val_1 + 1.5 \cdot feat_1 val_2 & -1 \cdot feat_2 val_1 + 1.5 \cdot feat_2 val_2 \end{bmatrix}$$

$$\boxed{errs = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}}$$

Gradient descent in linear algebra

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Gradient descent in linear algebra

Now all that we need to do is multiply with α/m and subtract from our old theta's:

$$\alpha/m \cdot \begin{bmatrix} -1\cdot 1+1.5\cdot 1 & -1\cdot feat_1val_1+1.5\cdot feat_1val_2 & -1\cdot feat_2val_1+1.5\cdot feat_2val_2 \end{bmatrix}$$
$$= \begin{bmatrix} \frac{\alpha}{m}(-1\cdot 1+1.5\cdot 1) & \frac{\alpha}{m}(-1\cdot feat_1val_1+1.5\cdot feat_1val_2) & \frac{\alpha}{m}(-1\cdot feat_2val_1+1.5\cdot feat_2val_2) \end{bmatrix}$$

Transpose it:

$$\begin{bmatrix} \frac{\alpha}{m}(-1\cdot 1+1.5\cdot 1) & \frac{\alpha}{m}(-1\cdot feat_1val_1+1.5\cdot feat_1val_2) & \frac{\alpha}{m}(-1\cdot feat_2val_1+1.5\cdot feat_2val_2) \end{bmatrix}^T = \begin{bmatrix} \frac{\alpha}{m}(-1\cdot 1+1.5\cdot 1) \\ \frac{\alpha}{m}(-1\cdot feat_1val_1+1.5\cdot feat_1val_2) \\ \frac{\alpha}{m}(-1\cdot feat_2val_1+1.5\cdot feat_2val_2) \end{bmatrix}$$

So finally:

$$\begin{bmatrix} \theta_{0old} \\ \theta_{1old} \\ \theta_{2old} \end{bmatrix} - \begin{bmatrix} \frac{\alpha}{m}(-1\cdot 1+1.5\cdot 1) \\ \boxed{\frac{\alpha}{m}(-1\cdot feat_1val_1+1.5\cdot feat_1val_2)} \\ \frac{\alpha}{m}(-1\cdot feat_2val_1+1.5\cdot feat_2val_2) \end{bmatrix} = \begin{bmatrix} \theta_{0new} \\ \theta_{1new} \\ \theta_{2new} \end{bmatrix}$$

$$\theta_{1new} = \theta_1 - \boxed{\frac{\alpha}{m}\sum_{i=1}^{m}\left(\left(h_\theta(x^{(i)}) - y^{(i)}\right)\cdot x_1^{(i)}\right)}$$

Logistic regression

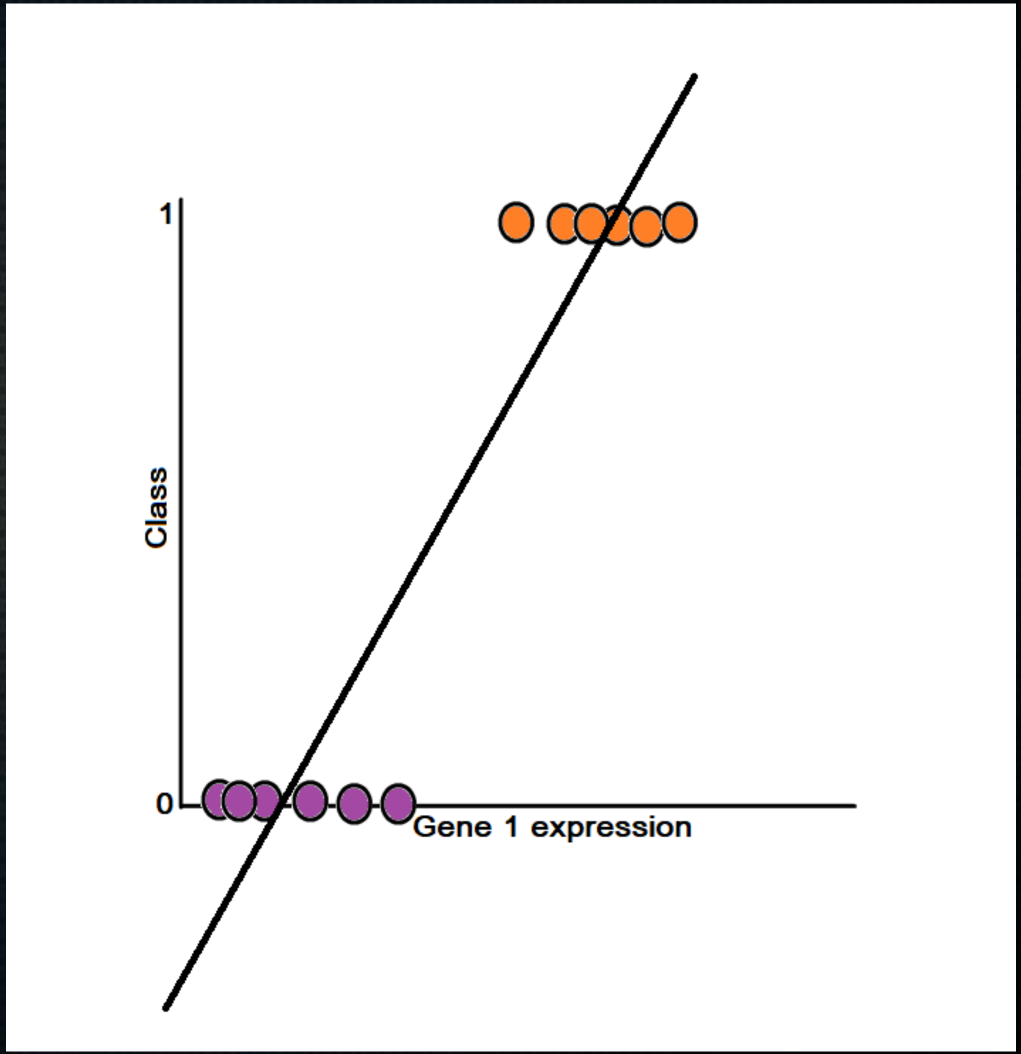
- You tell me: what is logistic regression?

Logistic regression

- Use regression-like framework for classification

Logistic regression

- Naïve idea:
  Train a linear regression. If Class >= 0.5, predict class 1. Otherwise, class 0.



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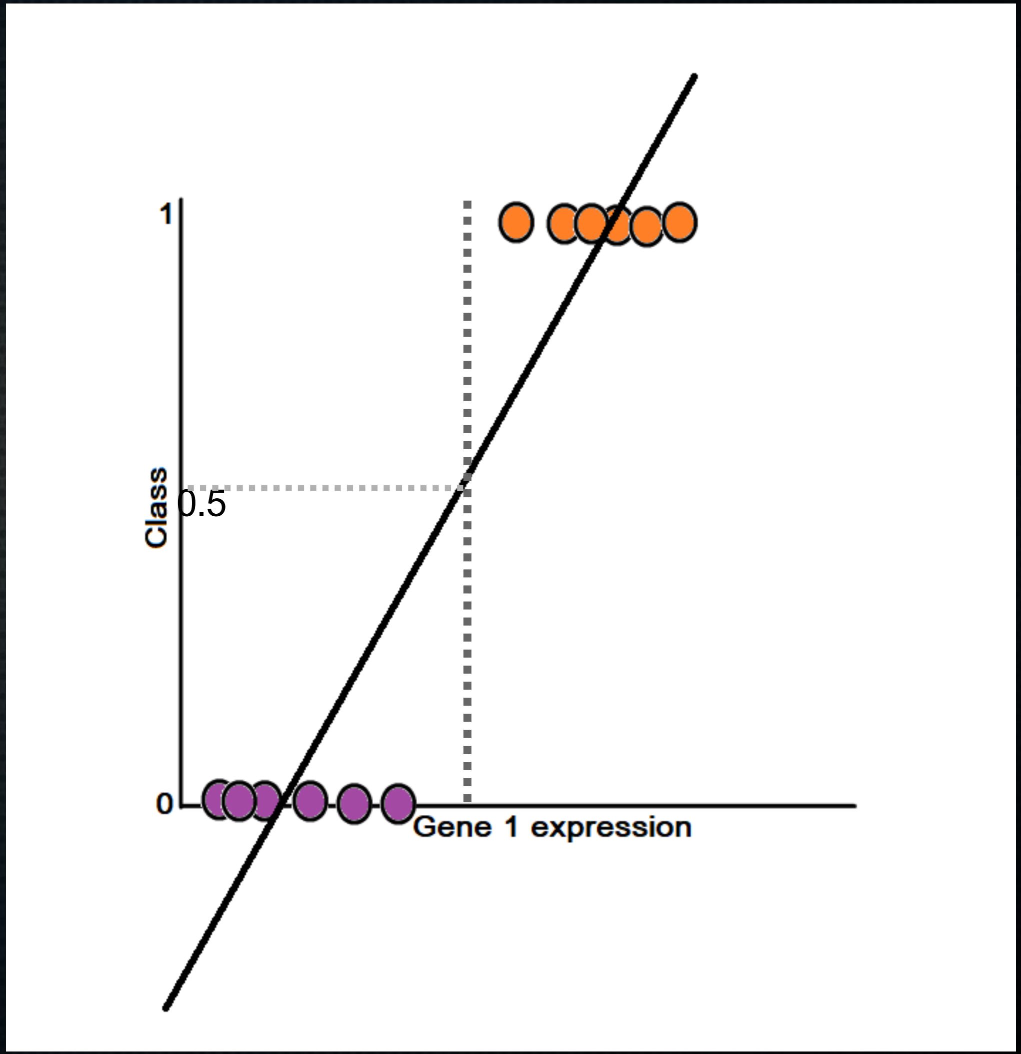

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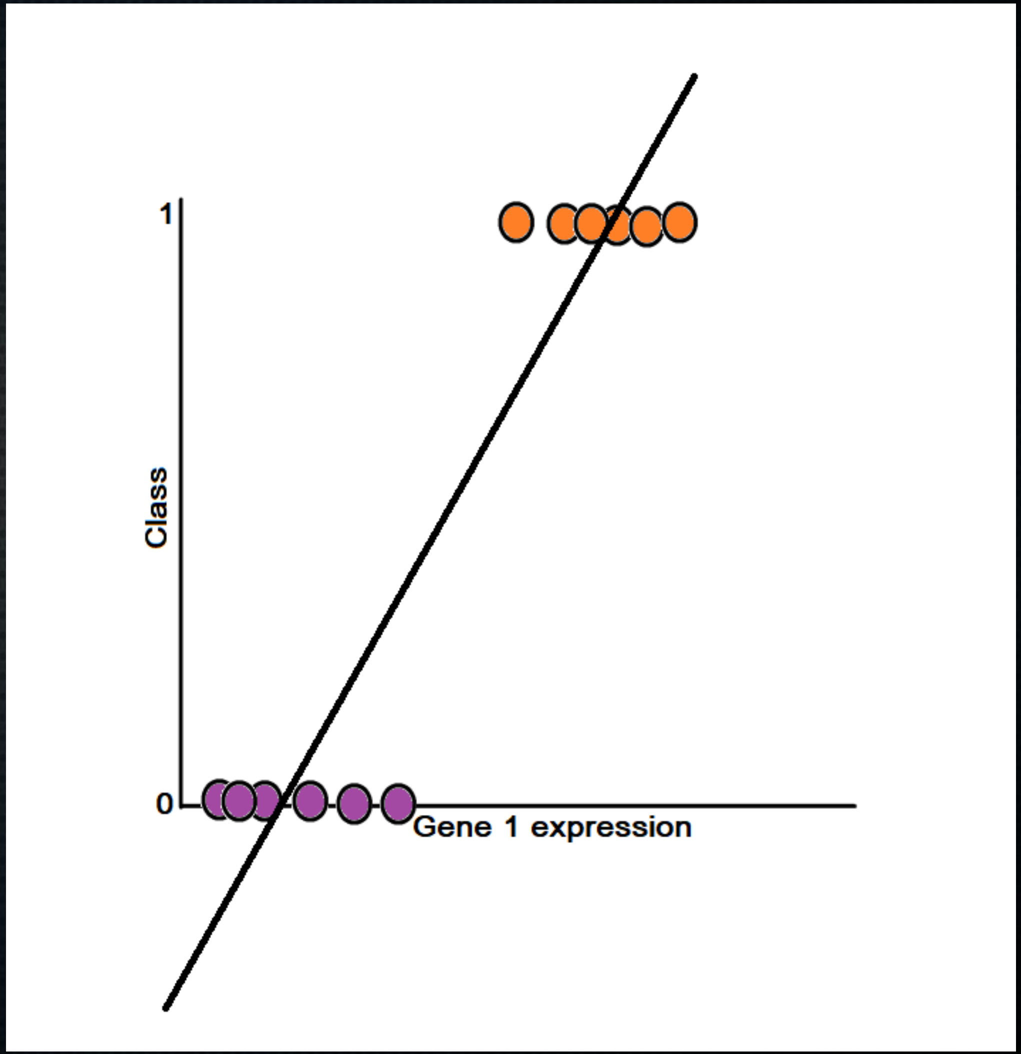
- Problems:
  -You can predict class > 1 and < 0, while that is not possible in reality.



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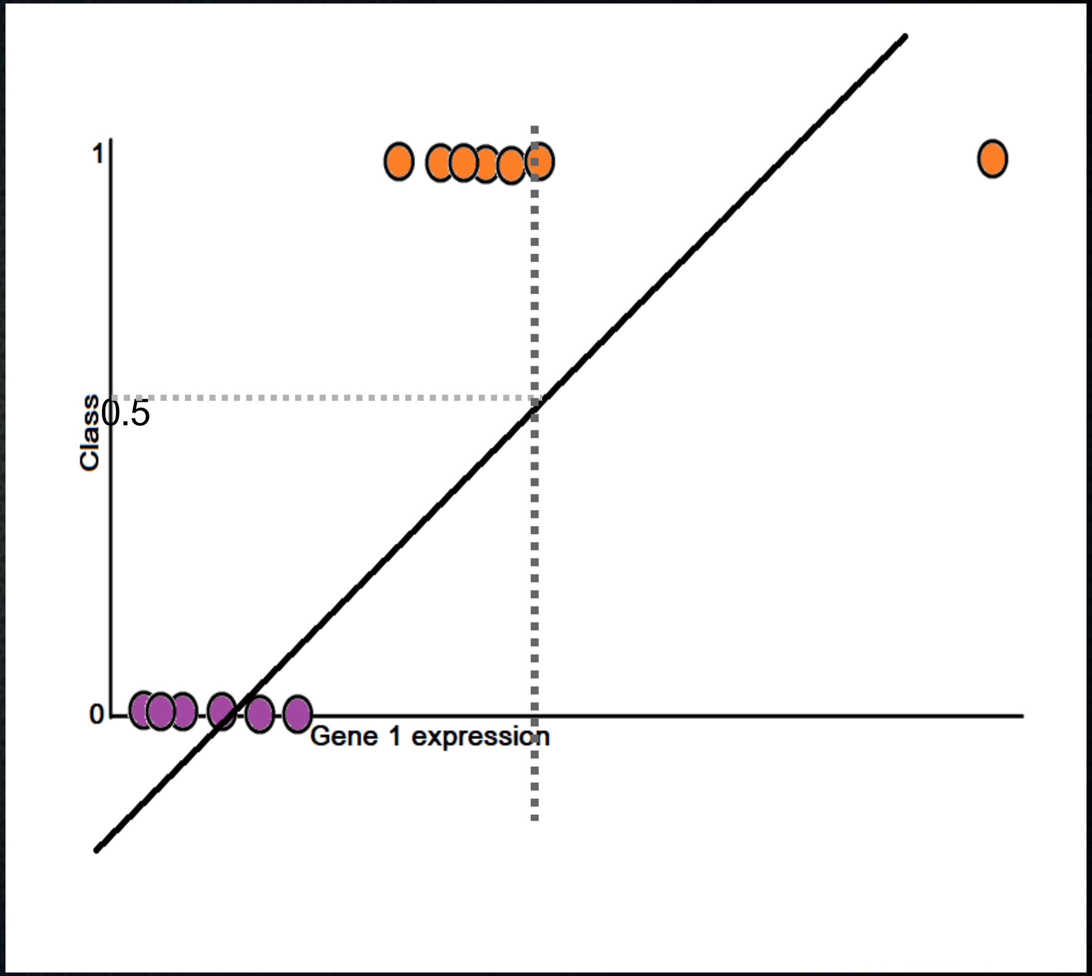

Logistic regression

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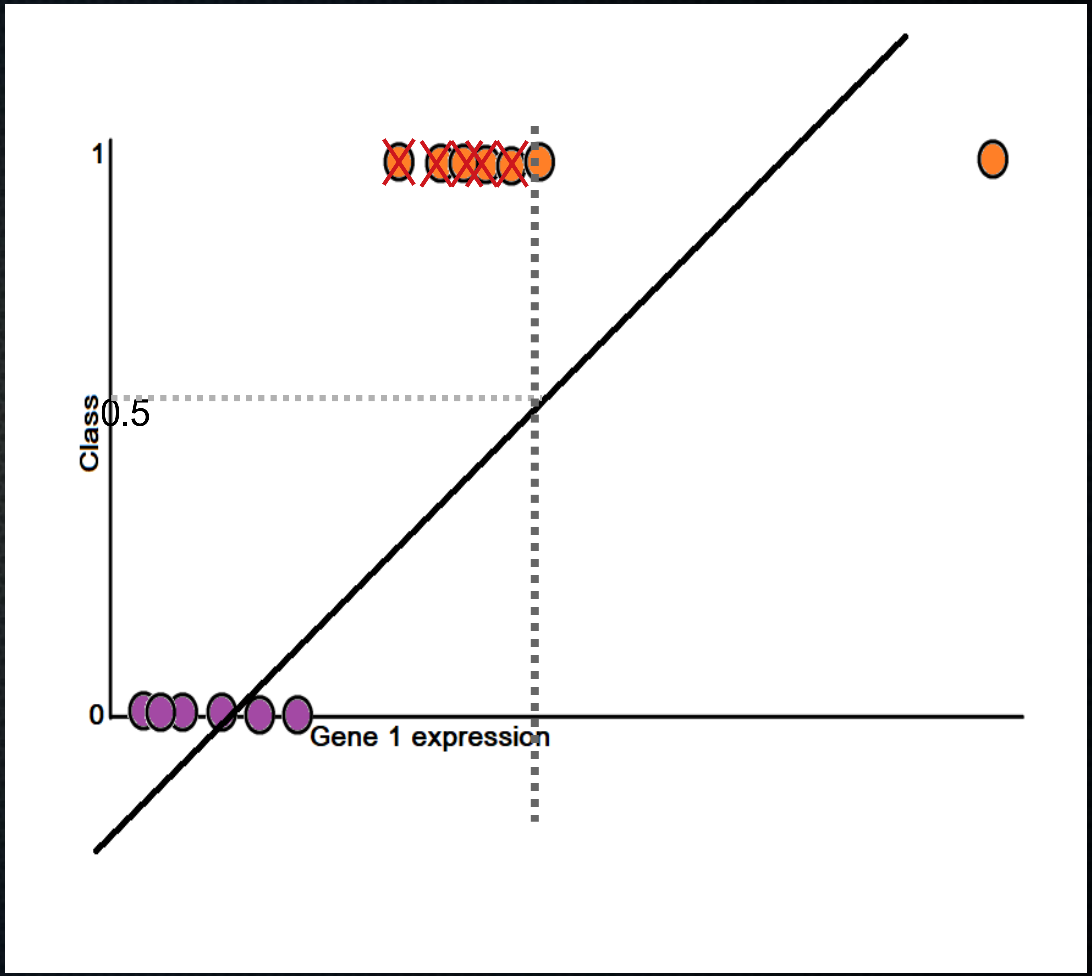
  -This example seemed to work, but quickly breaks down →
  get what is basically confirmation of hypothesis, but perform worse!



Logistic regression

- What we want:
  - Use the information that we only have two classes, 0 or 1.
  - Hypothesis function should output only numbers between 0 or 1.

Sigmoid or logistic function

- Before, our hypothesis function was of the form:

$$h_\theta(x) = \theta^T \cdot x$$

Sigmoid or logistic function

- Before, our hypothesis function was of the form:

$$h_\theta(x) = \theta^T \cdot x \longrightarrow [0.5 \;\; 3 \;\; -1.5] \cdot \begin{bmatrix} 1 \\ 3 \\ 8 \end{bmatrix}$$

Sigmoid or logistic function

- Before, our hypothesis function was of the form:

$$h_\theta(x) = \theta^T \cdot x \longrightarrow \underbrace{[0.5 \;\; 3 \;\; -1.5]}_{\text{Learned parameters (theta 0 – theta 2)}} \cdot \left.\begin{bmatrix}1\\3\\8\end{bmatrix}\right\} \text{Features for one sample (x0 = 1, intercept term, 2 data-derived features x1 and x2)}$$

Sigmoid or logistic function

- Before, our hypothesis function was of the form:

$$h_\theta(x)=\theta^T \cdot x \longrightarrow [0.5 \;\; 3 \;\; -1.5] \cdot \begin{bmatrix}1\\3\\8\end{bmatrix} = 0.5\cdot 1 + 3\cdot 3 - 1.5\cdot 8 = -2.5$$

Sigmoid or logistic function

- Before, our hypothesis function was of the form:

$$h_\theta(x) = \theta^T \cdot x$$

- Change that to the following:

$$h_\theta(x) = g(\theta^T \cdot x)$$

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- What does that look like?

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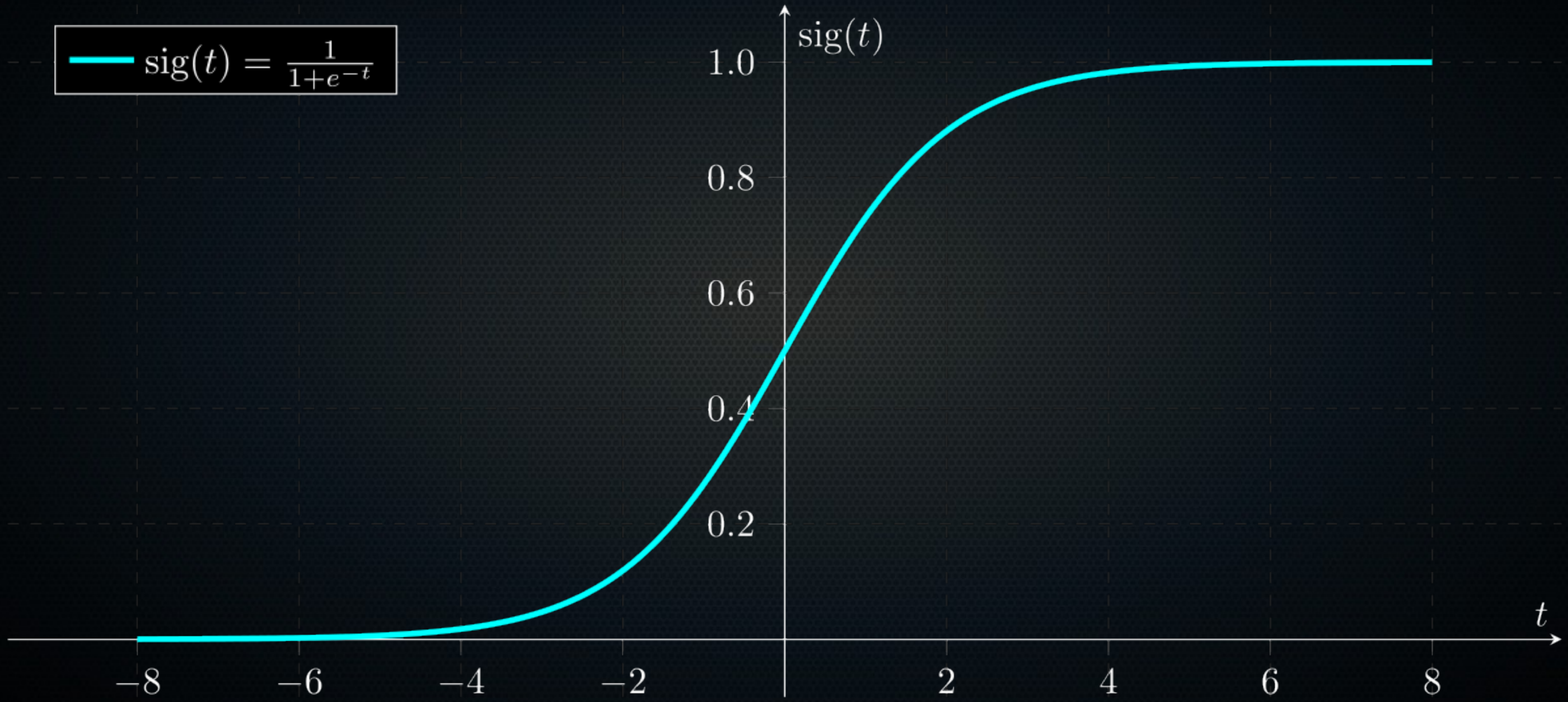
- What does that look like?

$$z \to \infty, e^{-z} \to 0$$

$$z \to -\infty, e^{-z} \to \infty$$

What does the sigmoid function look like?



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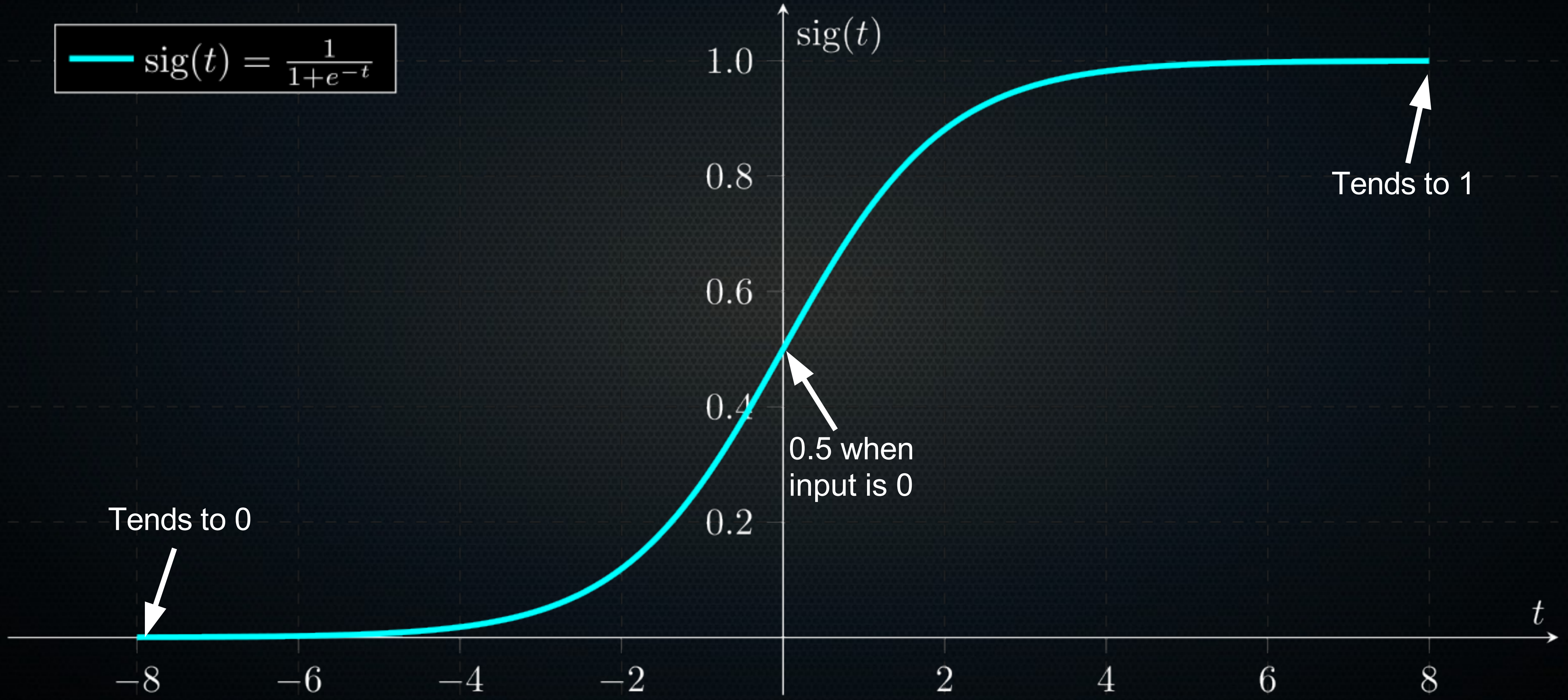
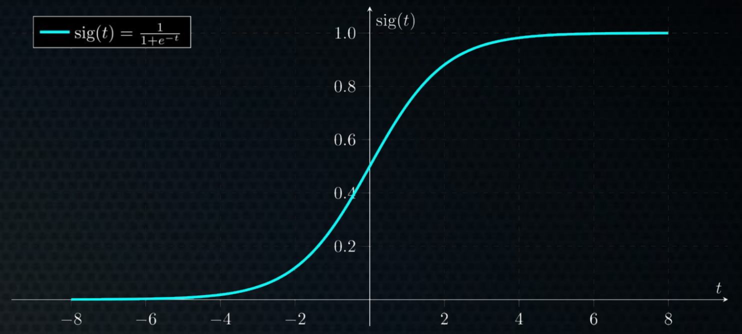


Sigmoid or logistic function

- How do we work with this? $h_\theta(x) = \frac{1}{1+e^{-(\theta^T \cdot x)}}$



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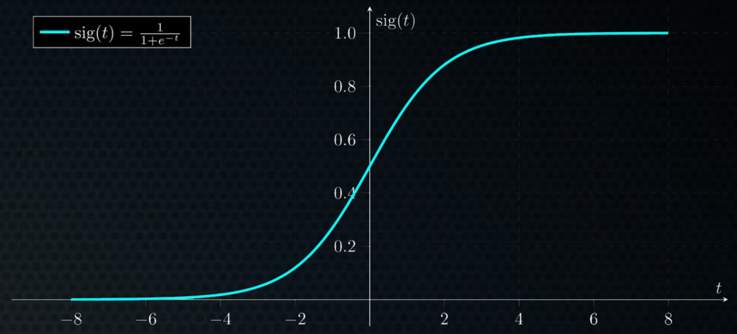
  - Interpret outcome of $h_\theta(x)$ as probability that class = 1 given the features.



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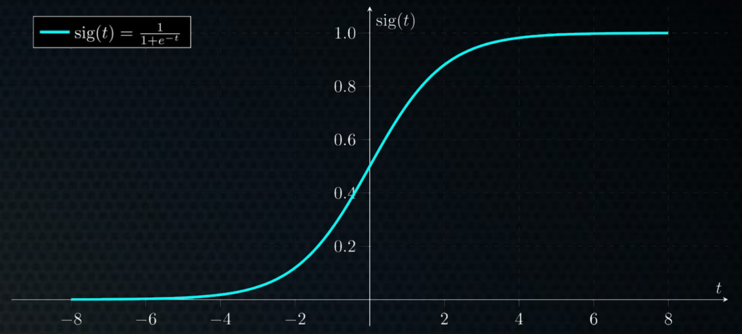

  - Interpret outcome of $h_\theta(x)$ as probability that class = 1 given the features. Example:

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{Tumor size} \\ \text{Neovascularisation level} \end{bmatrix}$$

$h_\theta(x) = 0.8 \longrightarrow$ 80% chance of tumor being malignant

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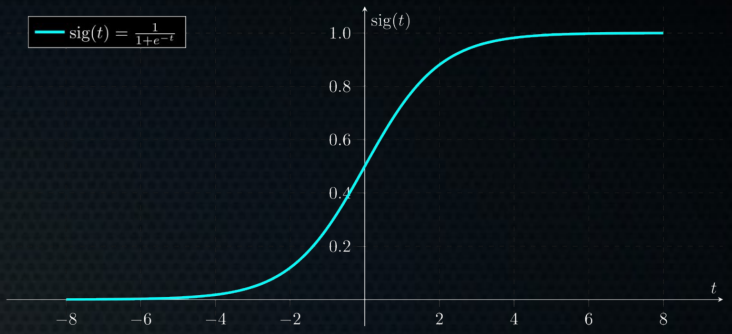

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$h_\theta(x) = 0.8 \longrightarrow$ 80% chance of tumor being malignant (class 1)

100% - 80% → 20 % chance of being benign (class 0)

Sigmoid or logistic function

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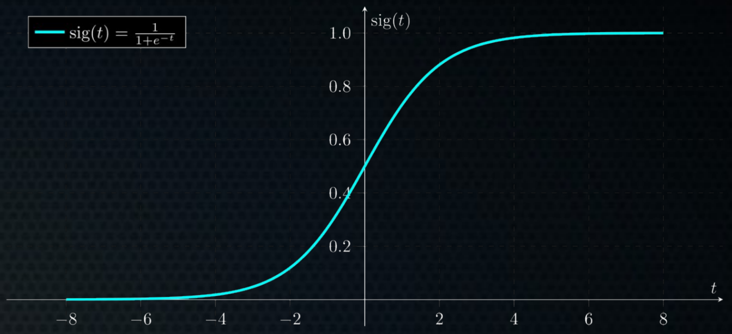

  - Interpret outcome of $h_\theta(x)$ as probability that class = 1 given the features.
  - Formally:

$$h_\theta(x) = \frac{1}{1+e^{-(\theta^T \cdot x)}} = p(y=1|x;\theta)$$

$$p(y=0|x;\theta) = 1 - h_\theta(x)$$

Sigmoid or logistic function

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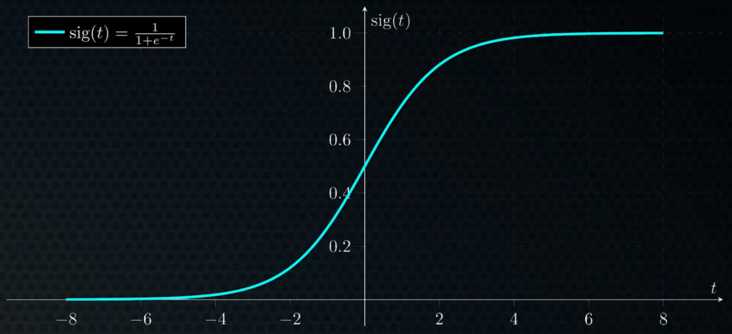


$$\left.\begin{aligned} h_\theta(x) &= \frac{1}{1+e^{-(\theta^T \cdot x)}} = p(y=1|x;\theta) \\ p(y=0|x;\theta) &= 1-h_\theta(x) \end{aligned}\right\} \frac{p(y=1)}{1-p(y=1)}$$

Log odds

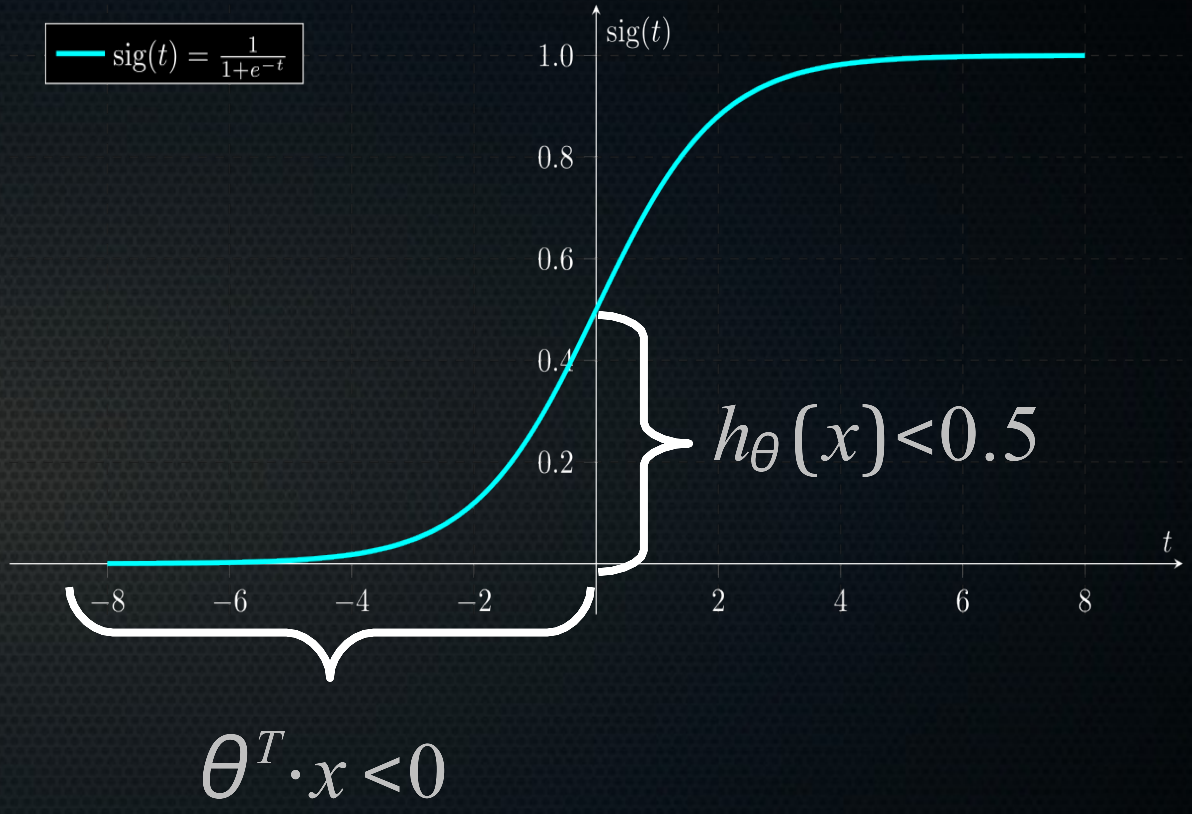
Coefficients:

	Estimate	Std. Error	z value	Pr(>|z|)	
(Intercept)	-8.922213	0.879485	-10.145	< 2e-16	***
pregnant	0.106275	0.039885	2.665	0.00771	**
glucose	0.036555	0.004546	8.041	8.88e-16	***
pressure	-0.008019	0.006230	-1.287	0.19801	
triceps	0.001909	0.008258	0.231	0.81721	
insulin	-0.001394	0.001098	-1.269	0.20445	
mass	0.082665	0.017927	4.611	4.00e-06	***
pedigree	0.901691	0.374350	2.409	0.01601	*
age	0.020417	0.010854	1.881	0.05995	.

logOdds(diabetes) = -8.9 + (0.106*pregnant) + (0.037*glucose).... + (0.02*age)

Decision boundary

- Threshold:



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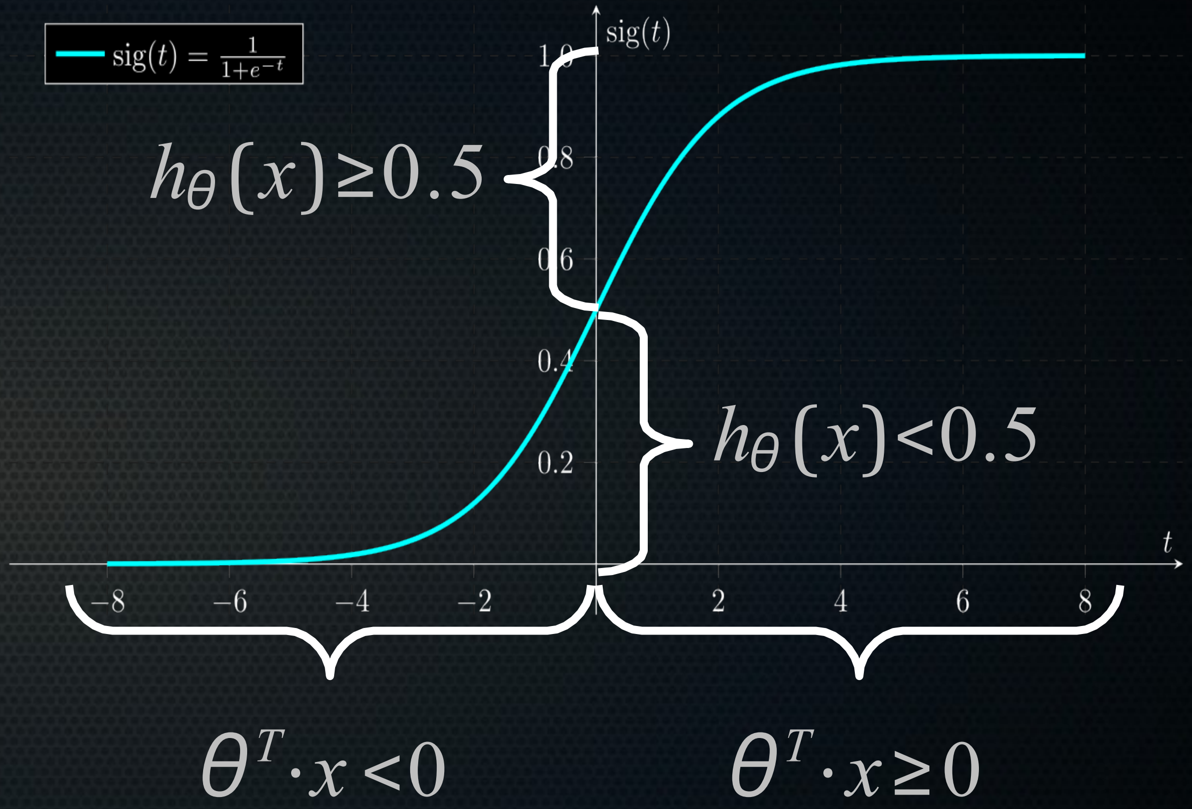
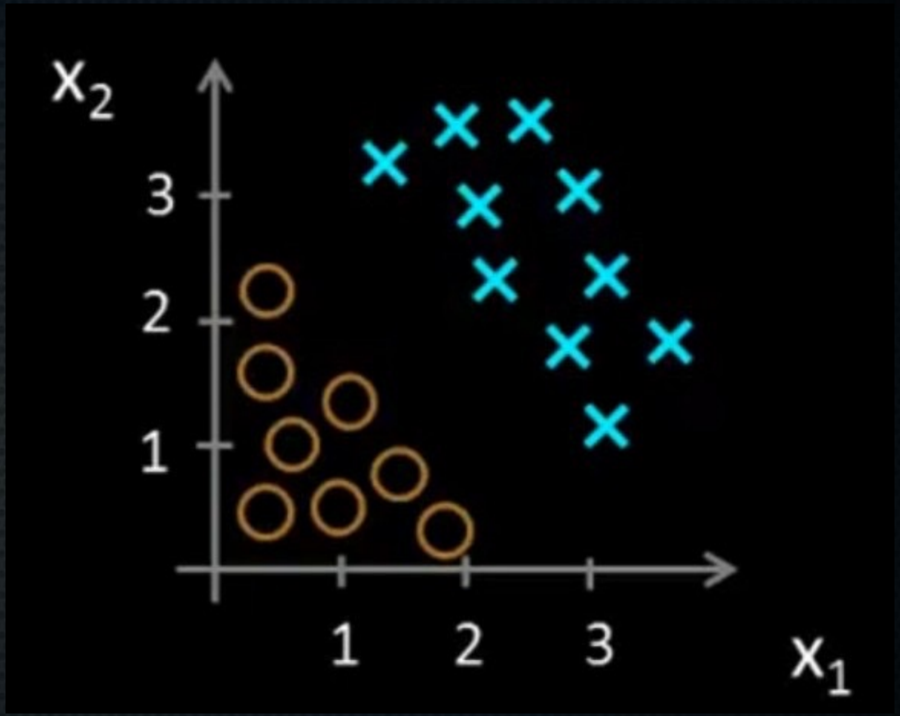


Decision boundary

- How does it look?

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

$$h_\theta(x)=g(\theta_0 \cdot x_0, \theta_1 \cdot x_1, \theta_2 \cdot x_2)$$



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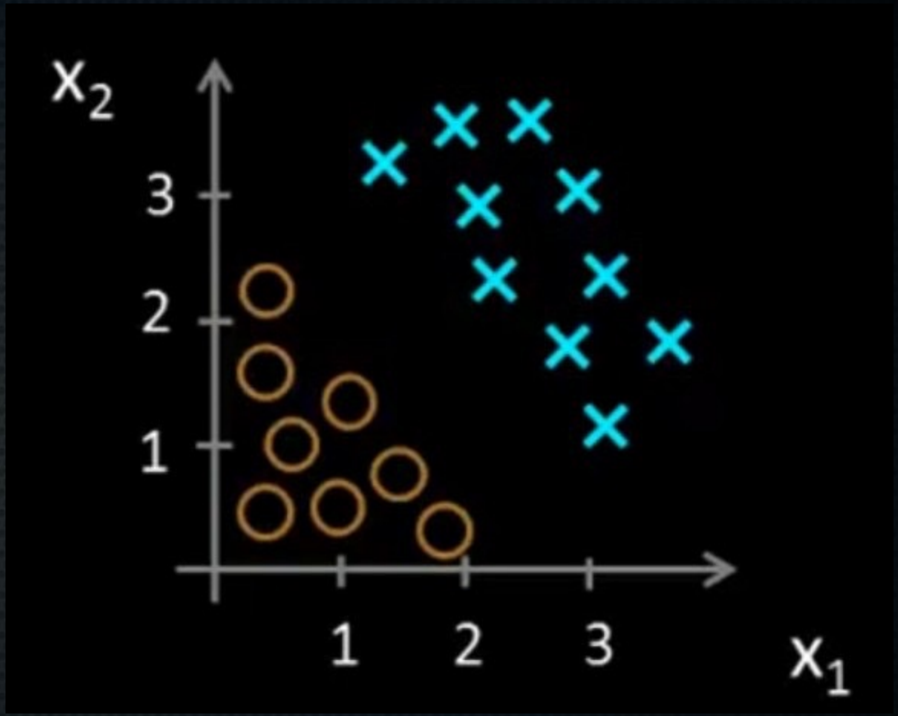
$$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$$



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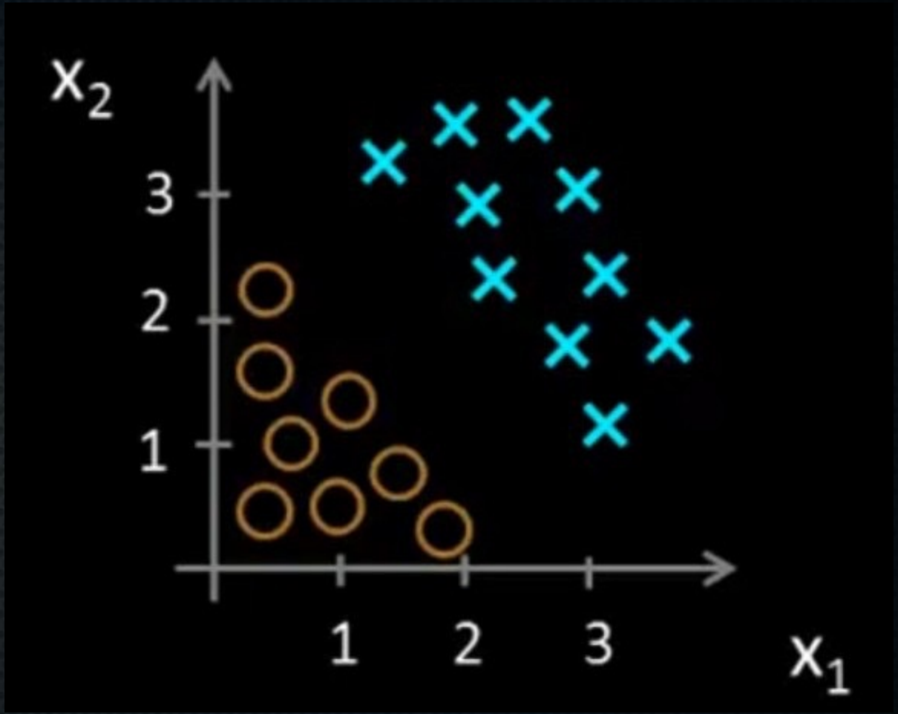
$$\underbrace{\theta=\begin{bmatrix}-3\\1\\1\end{bmatrix}}_{y=1 \text{ if} -3\cdot 1+1\cdot x_1+1\cdot x_2\geq 0}$$



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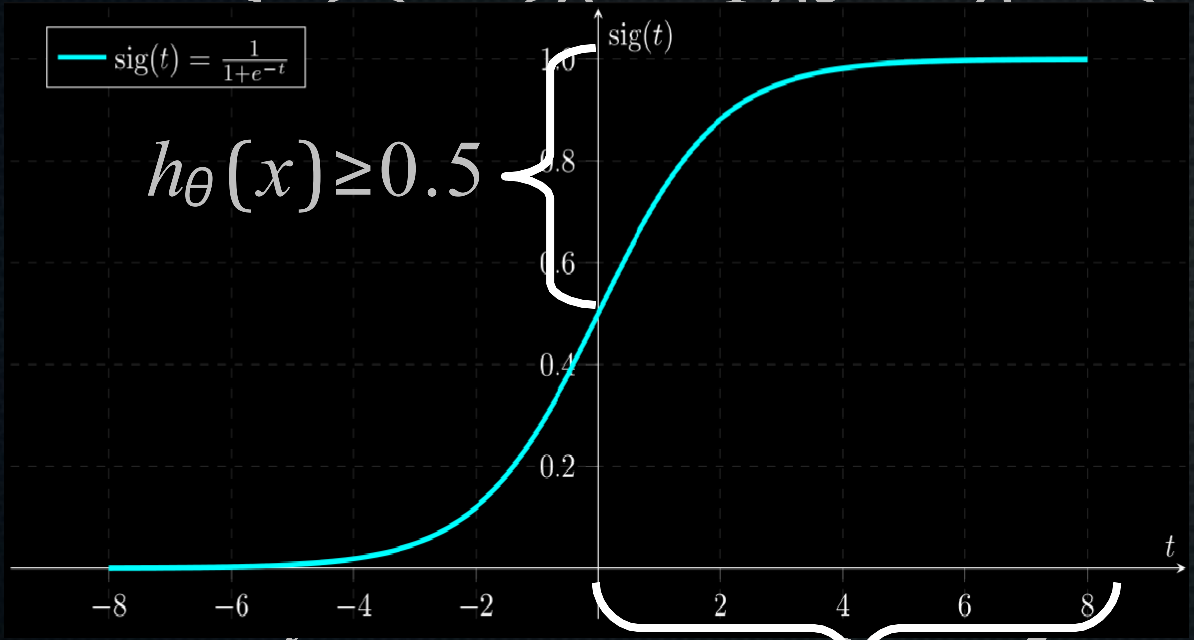
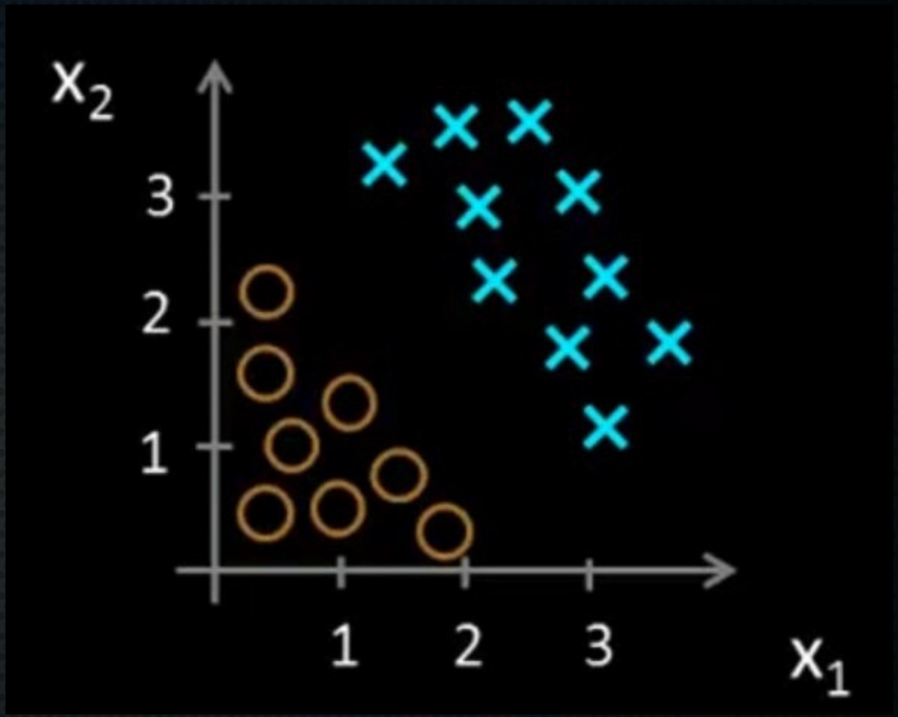


$h_\theta(x) \geq 0.5$

$\theta^T \cdot x \geq 0$



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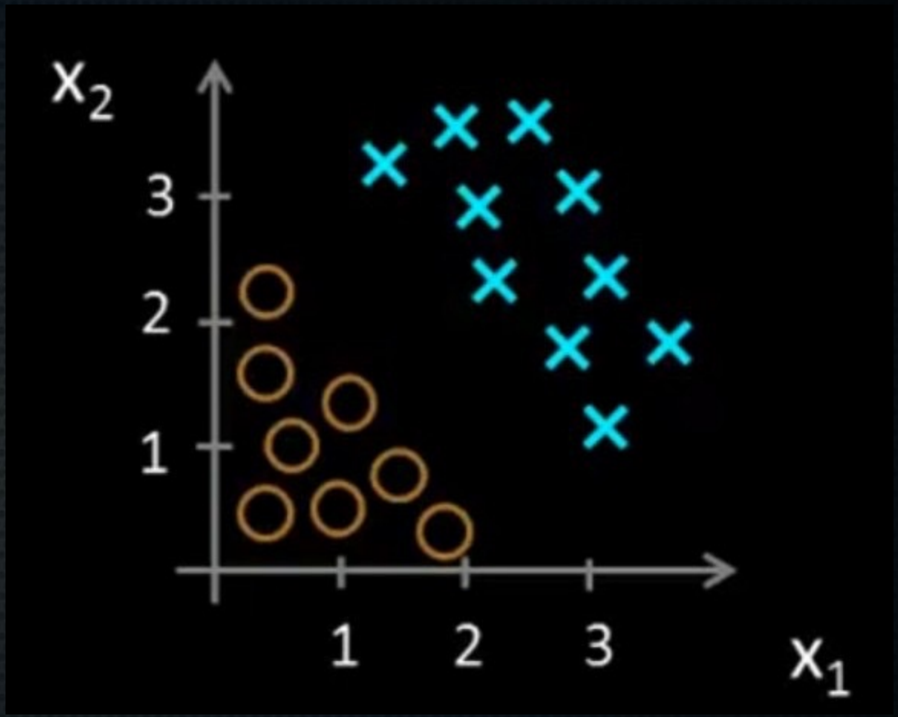
$$x_1+x_2=3$$



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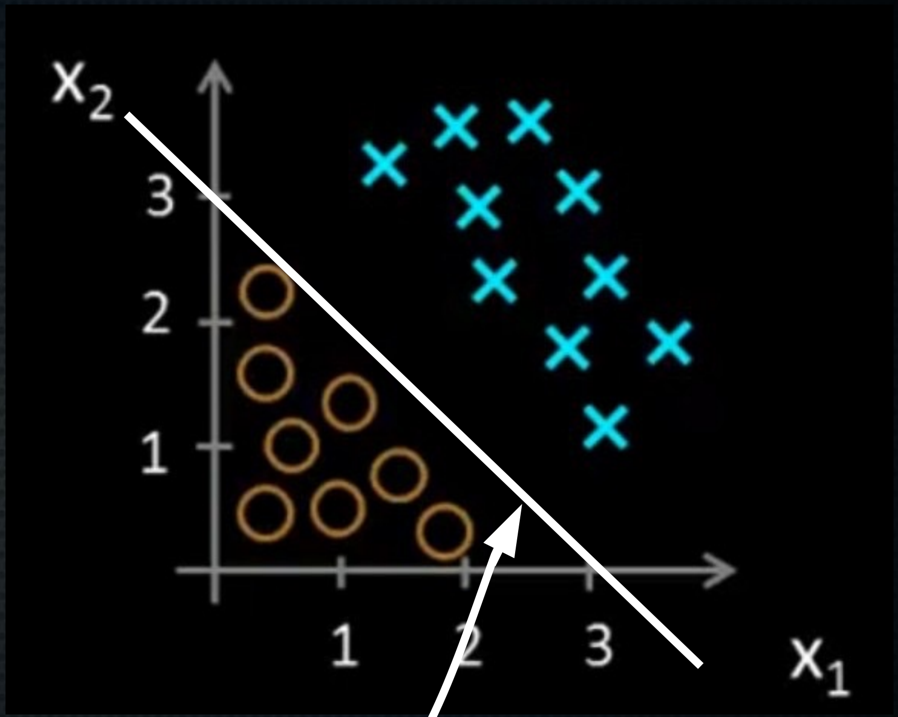

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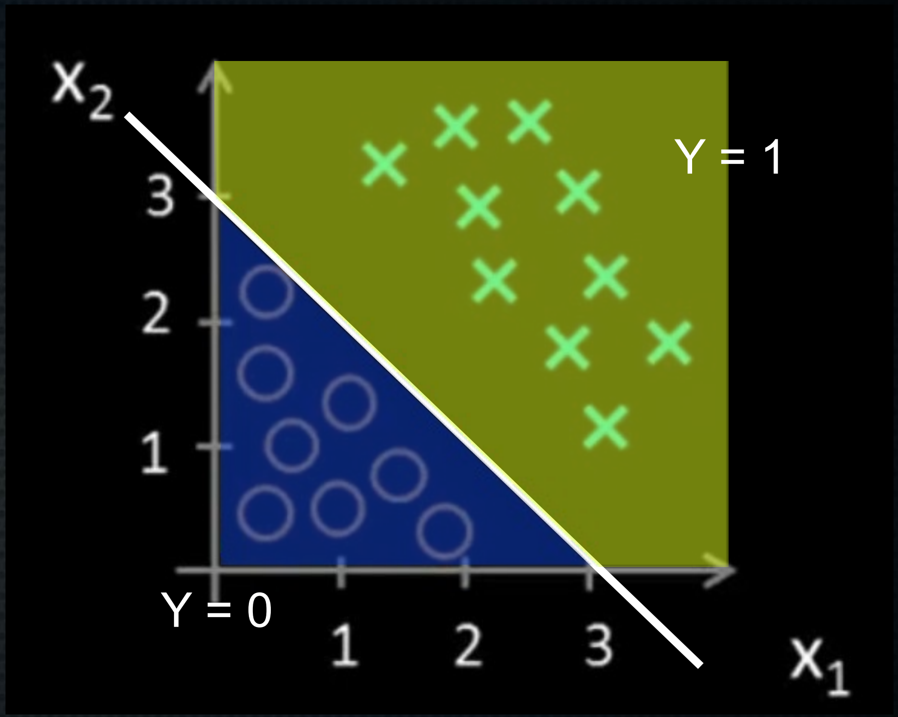

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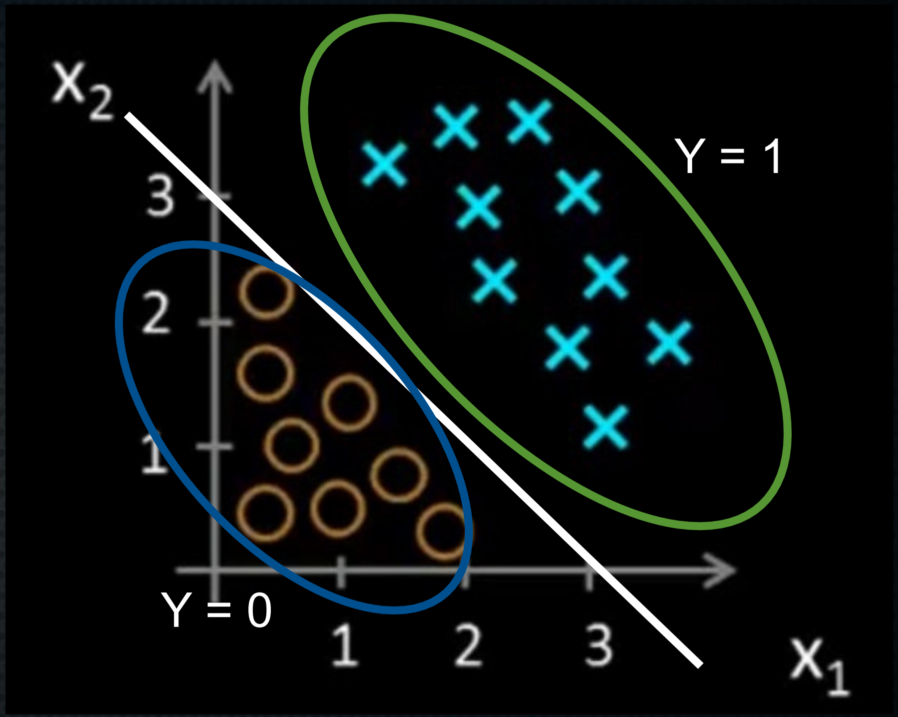

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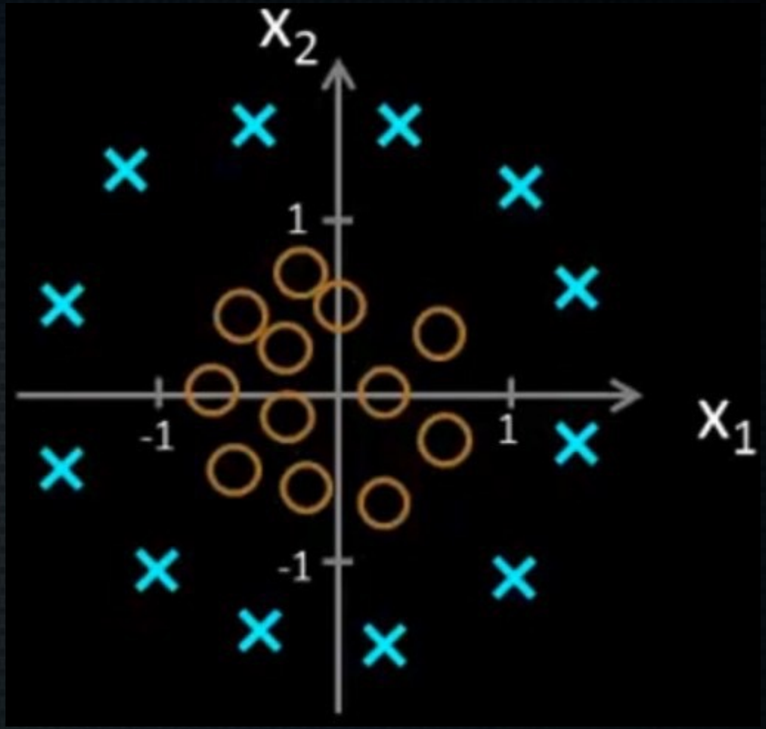


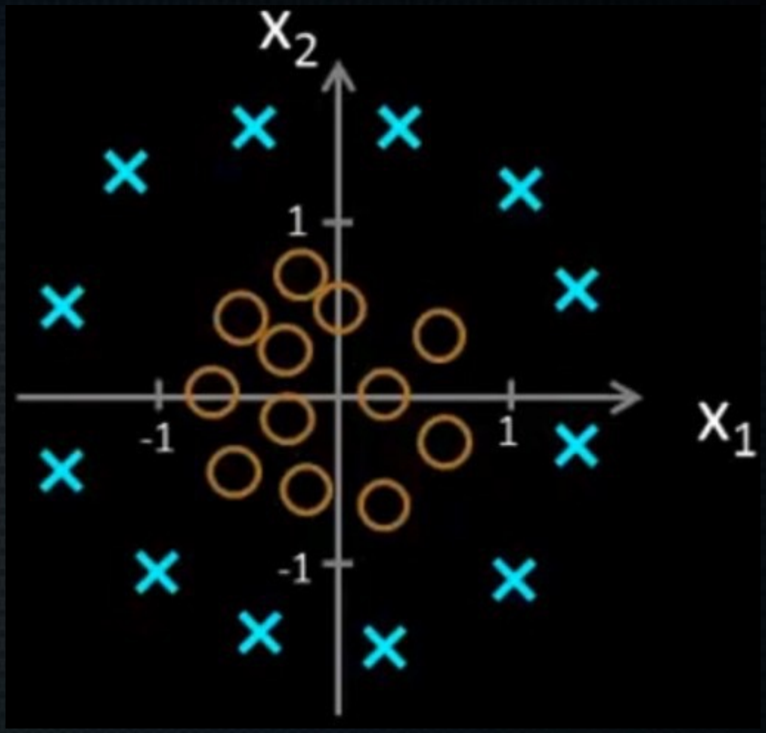
$$y=1 \text{ if} -3 \cdot 1 + 1 \cdot x_1 + 1 \cdot x_2 \geq 0$$

Non-linear decision boundary

- How does it look? $g(z)=\frac{1}{1+e^{-z}}$

$$h_\theta(x)=g(\theta_0 x_0,\theta_1 x_1,\theta_2 x_2,\boxed{\theta_3 x_1^2,\theta_4 x_2^2})$$

- Add two polynomial features



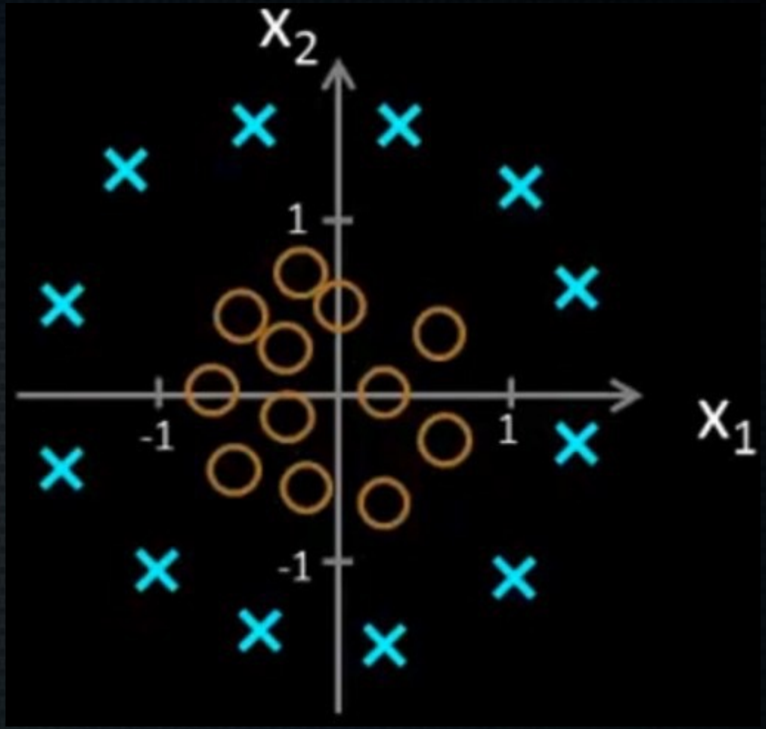
Non-linear decision boundary

- How does it look? $g(z)=\dfrac{1}{1+e^{-z}}$

$$h_\theta(x)=g(\theta_0 x_0,\theta_1 x_1,\theta_2 x_2,\boxed{\theta_3 x_1^2,\theta_4 x_2^2})$$

- Add two polynomial features

$$\theta=\begin{bmatrix}-1\\0\\0\\1\\1\end{bmatrix}$$



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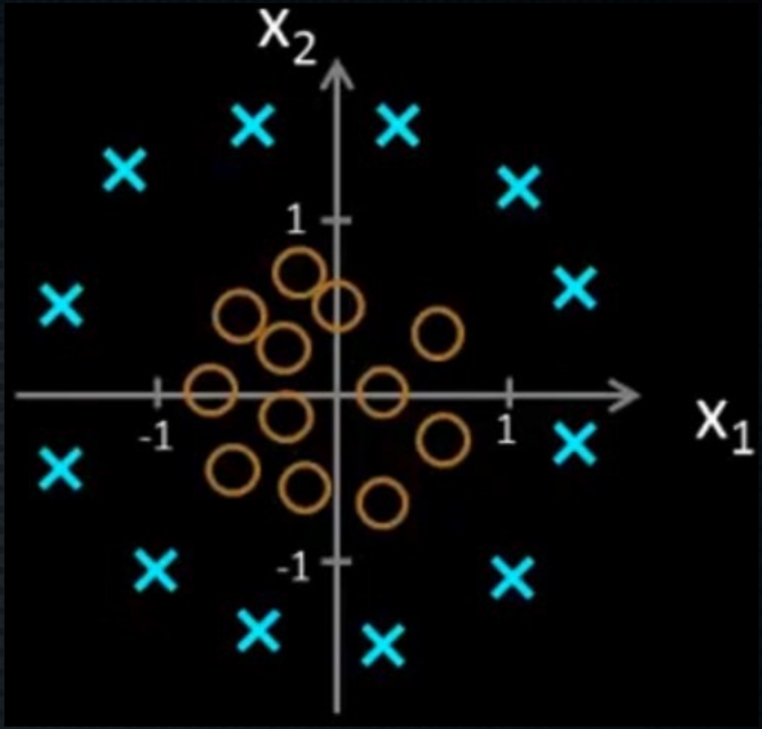
Can you work out what the decision boundary will be?



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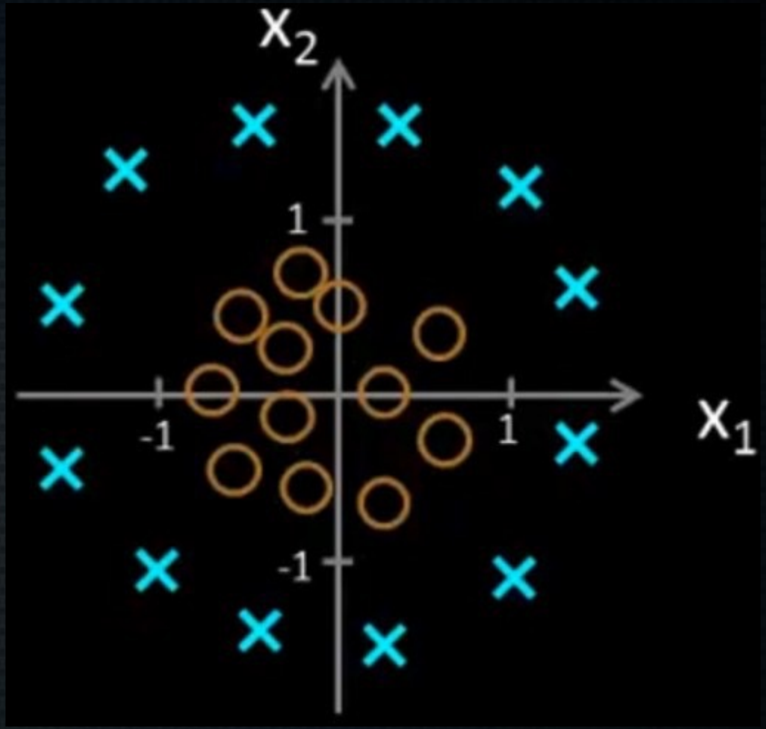

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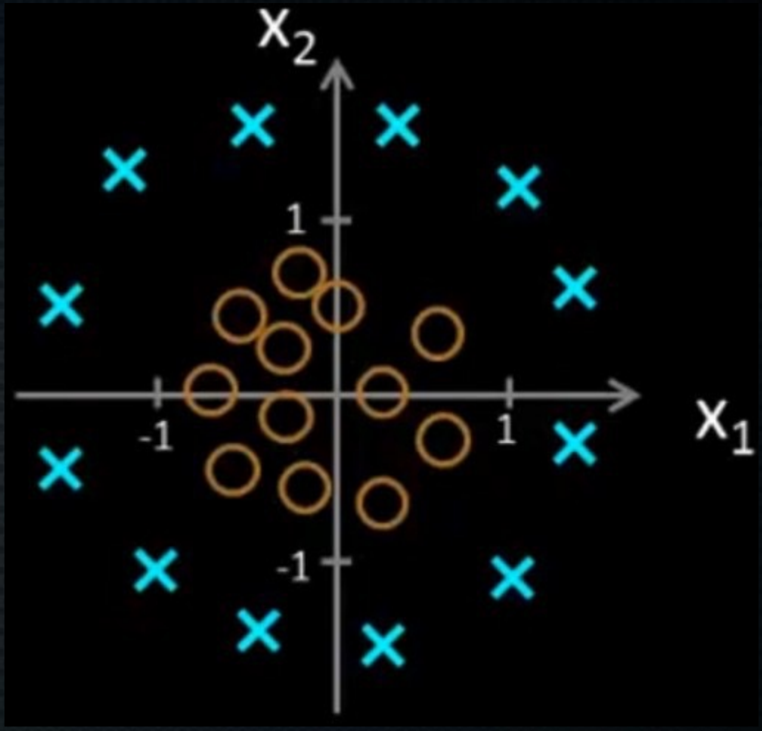

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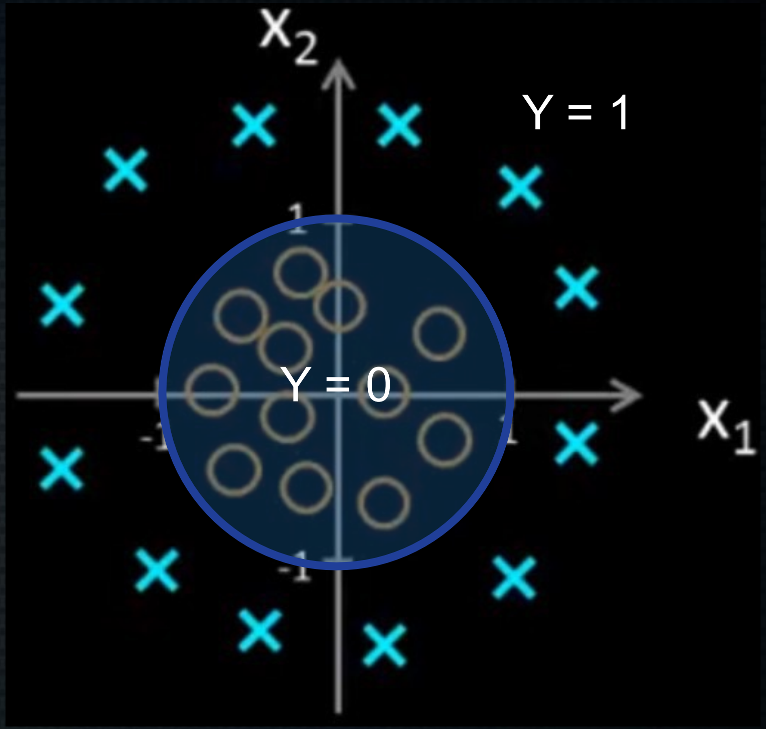
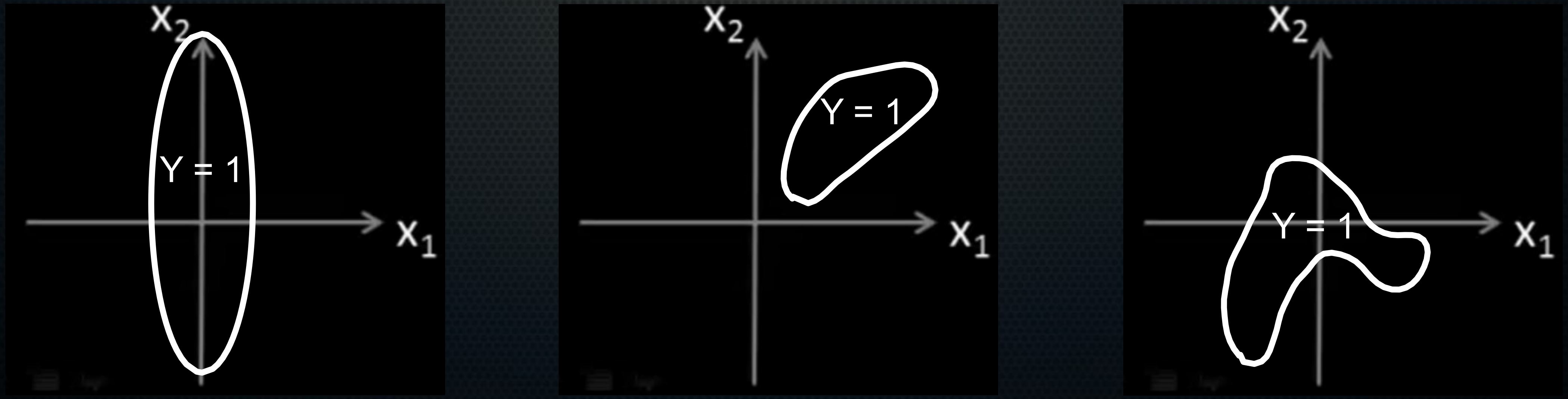


Non-linear decision boundary

- How does it look?
- If you add more and higher-order polynomial features, you can get complex boundaries:



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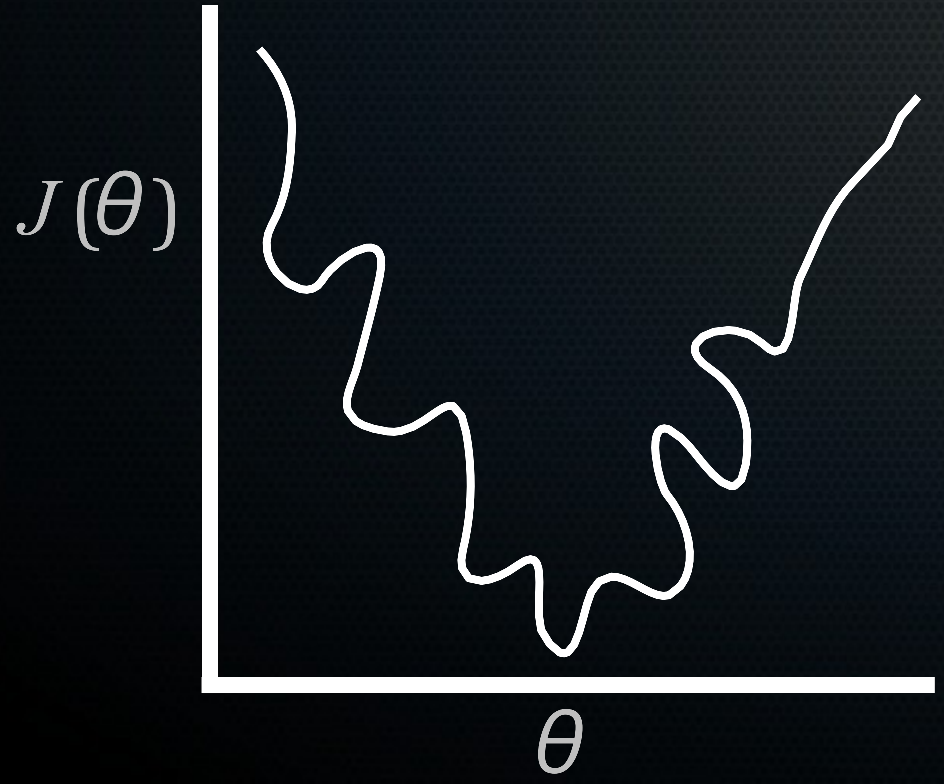

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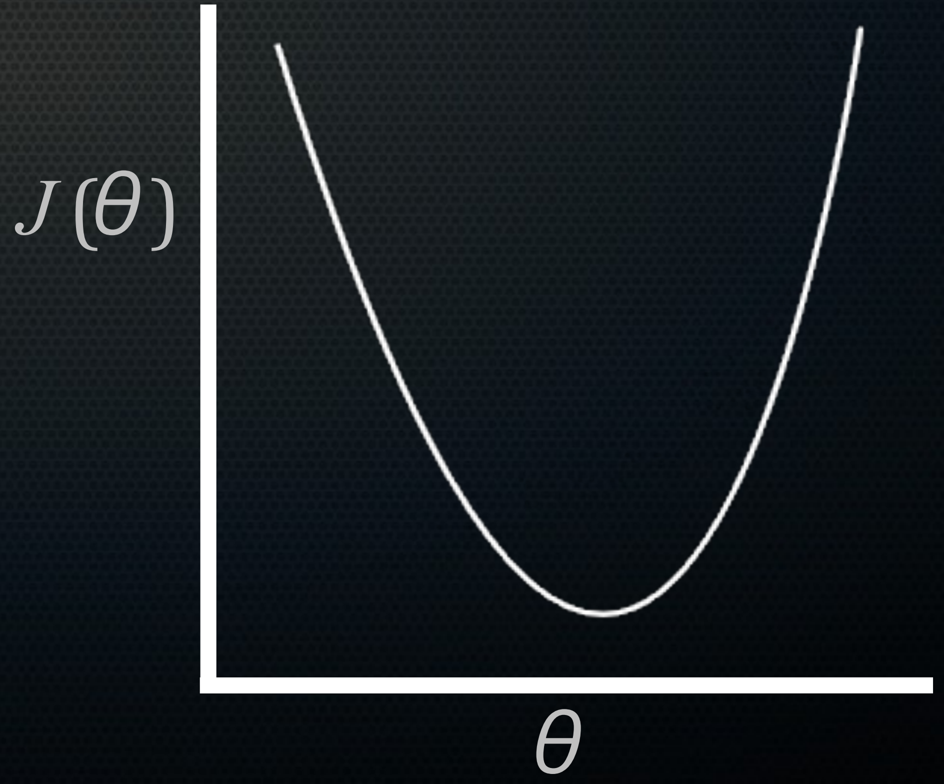

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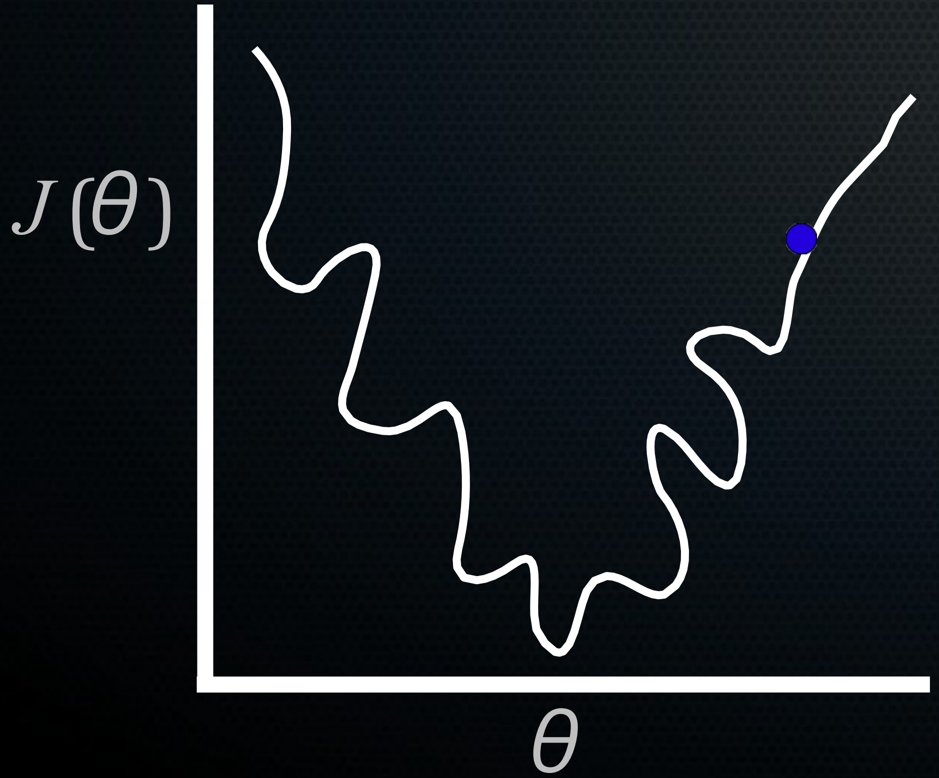

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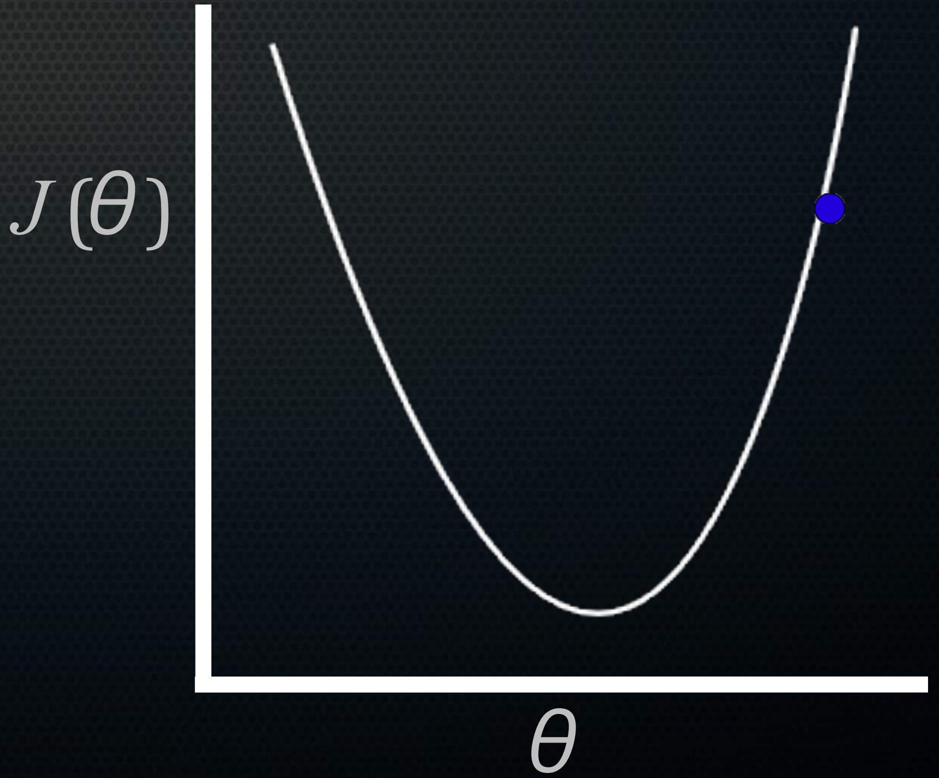

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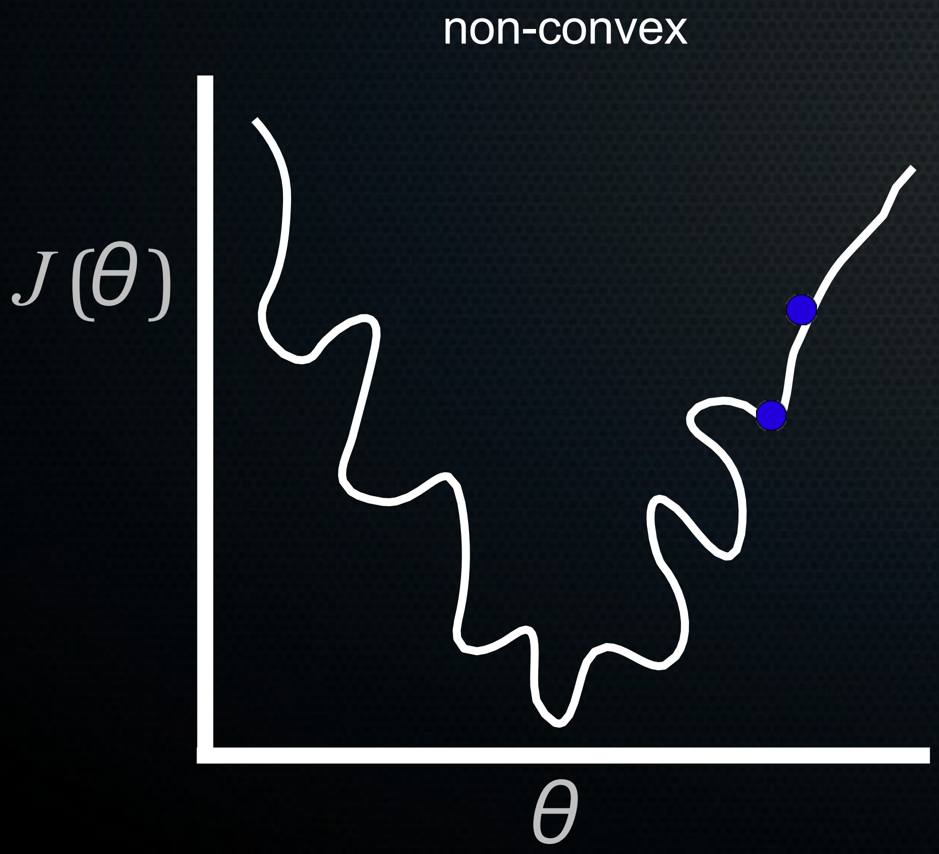

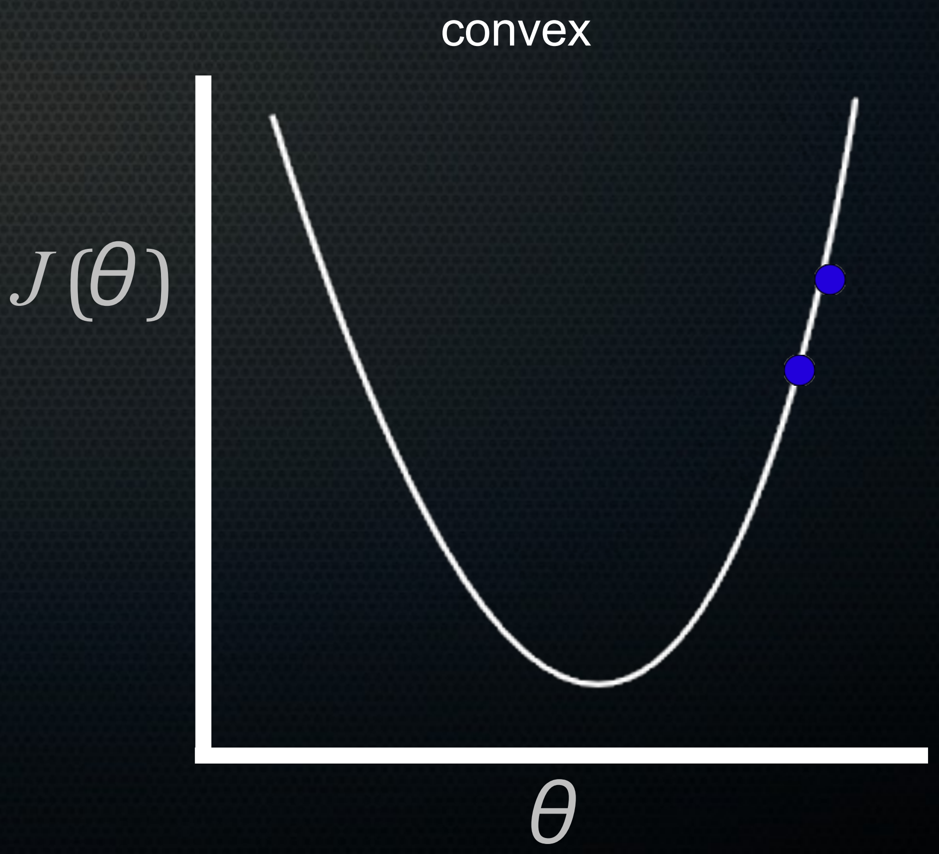

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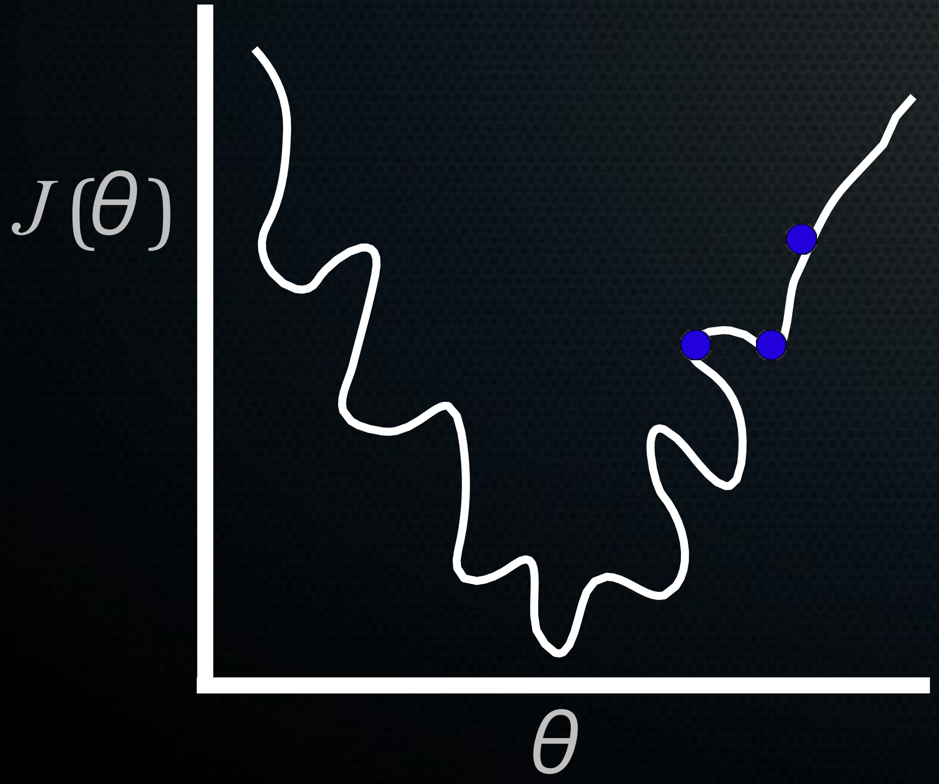

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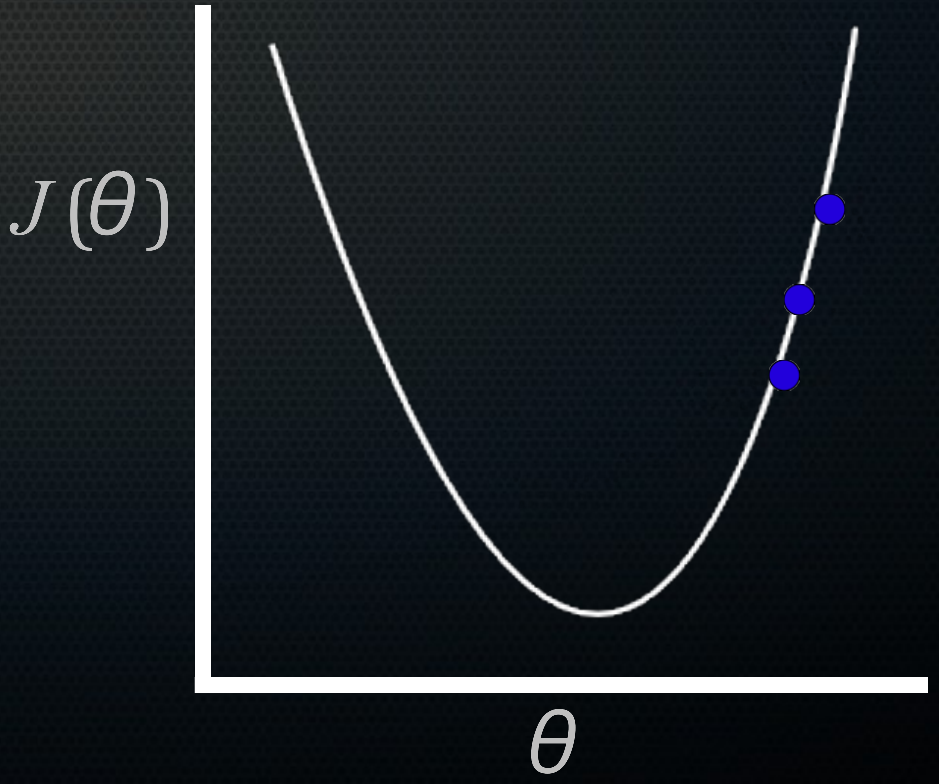

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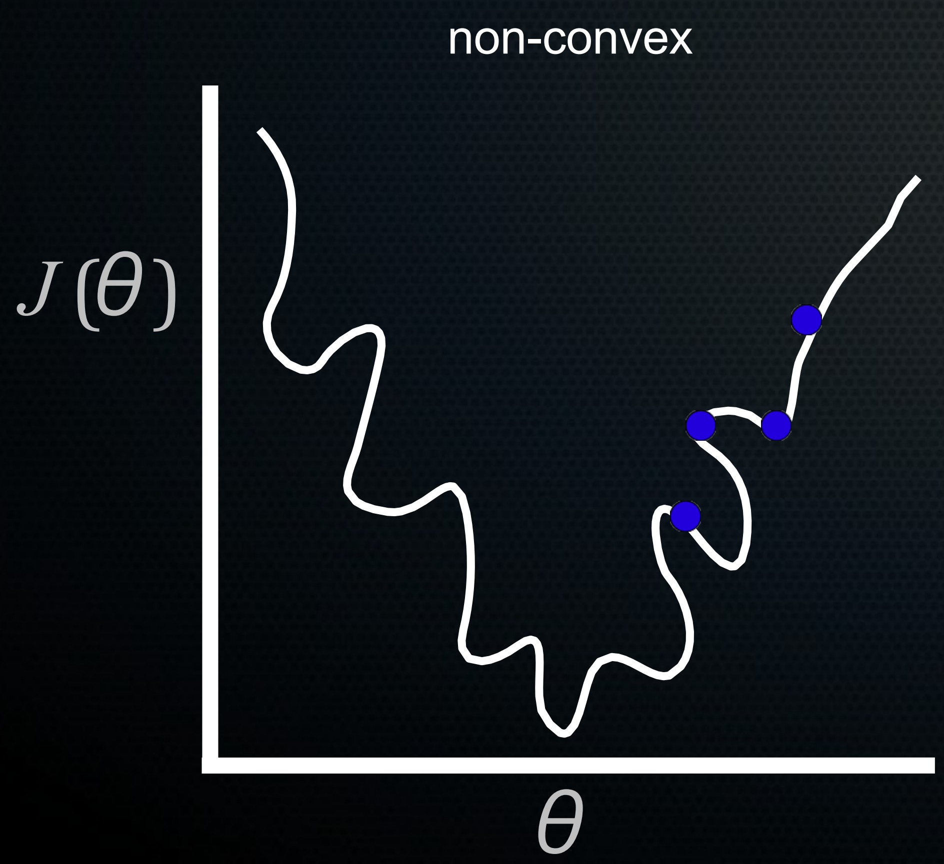

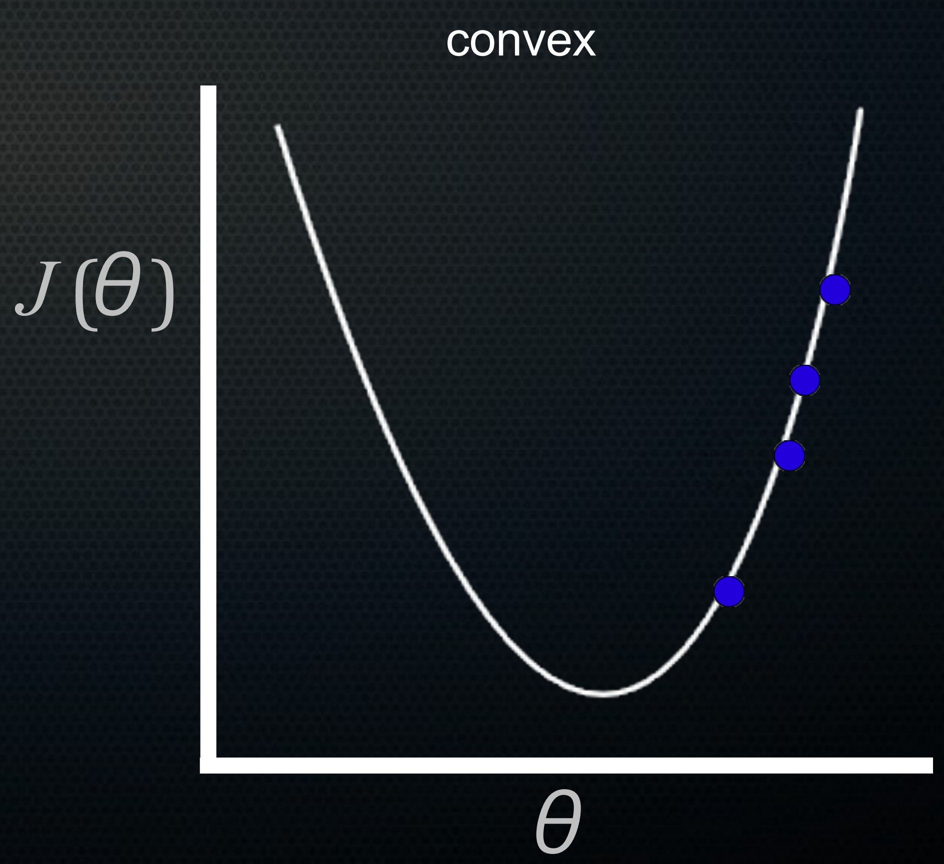

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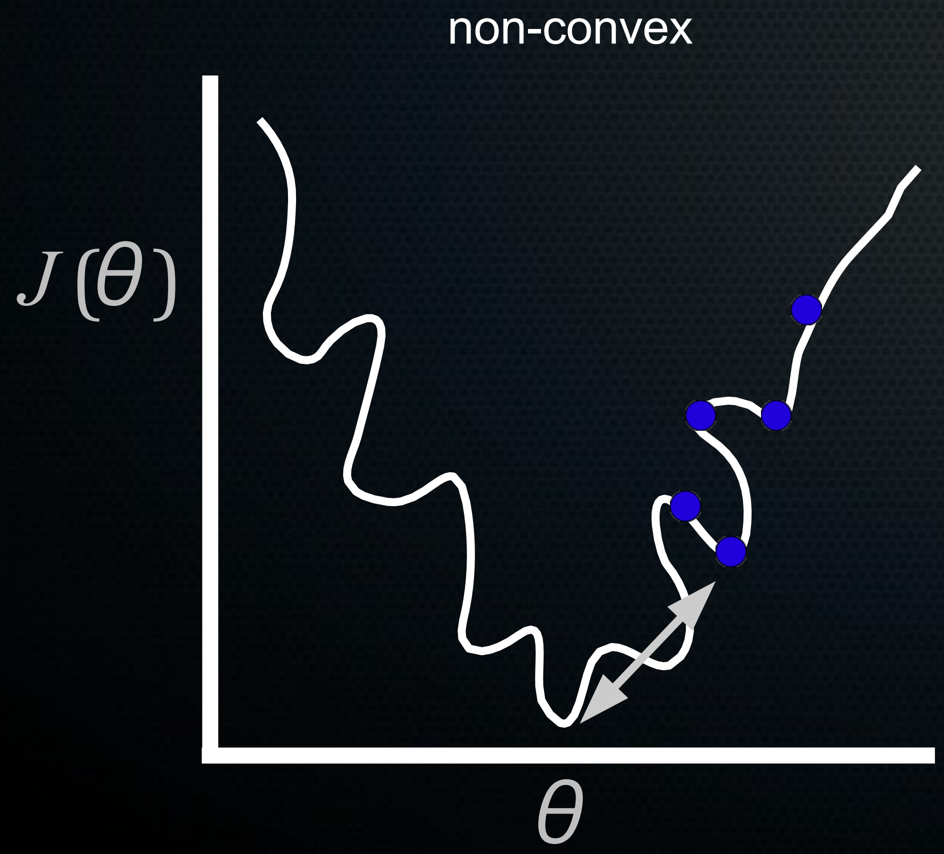

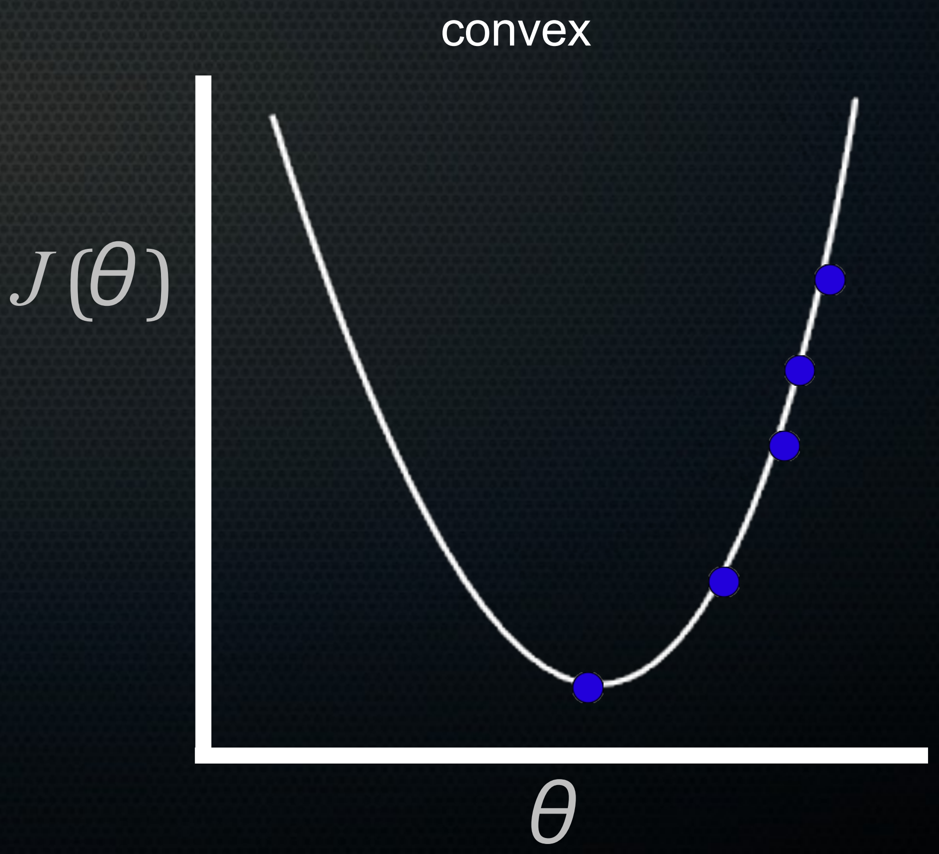

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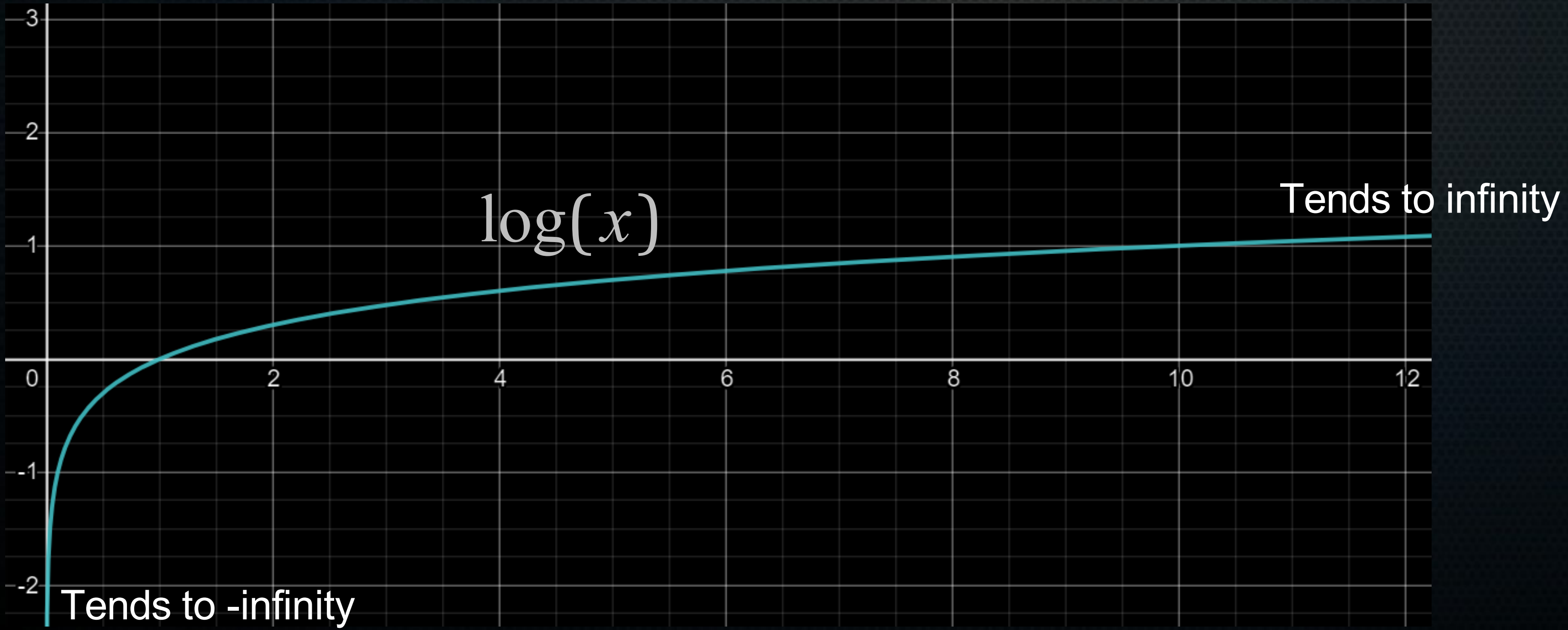

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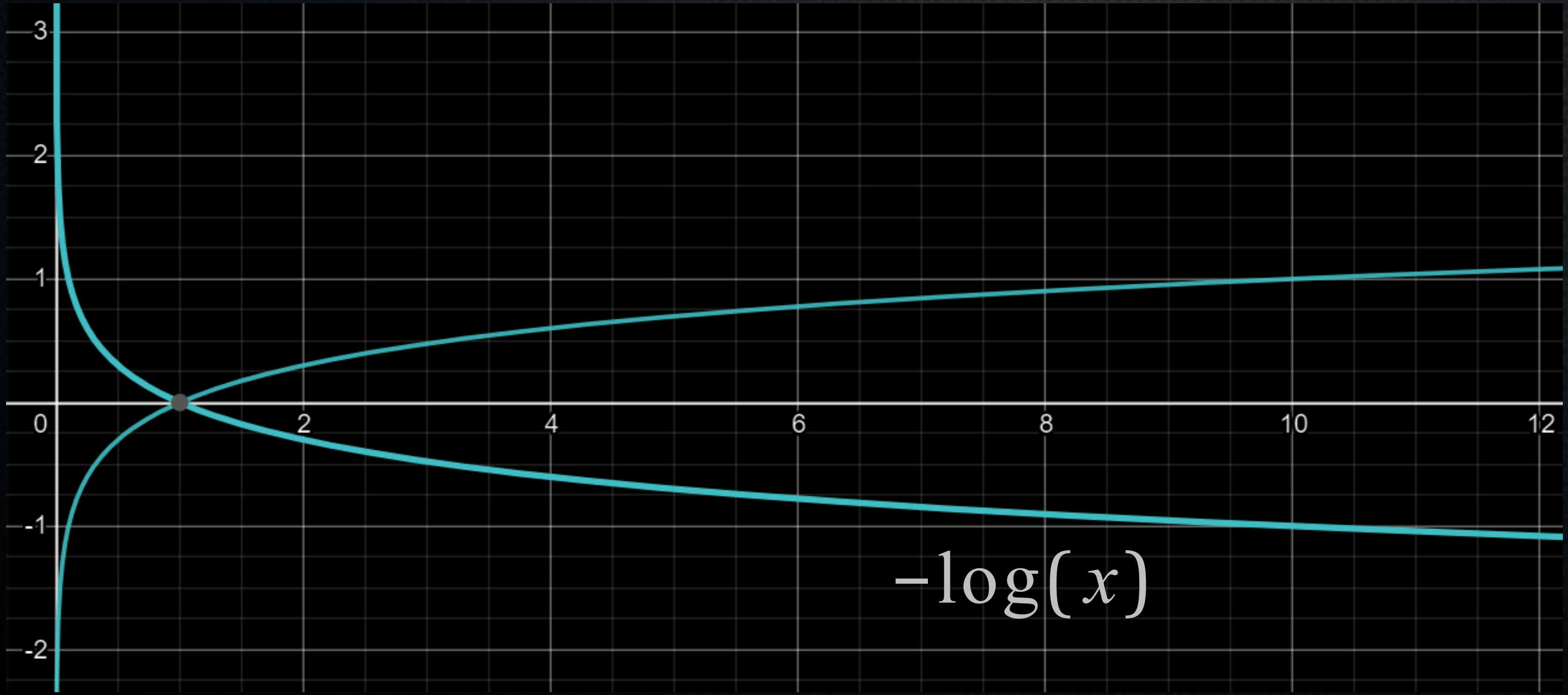

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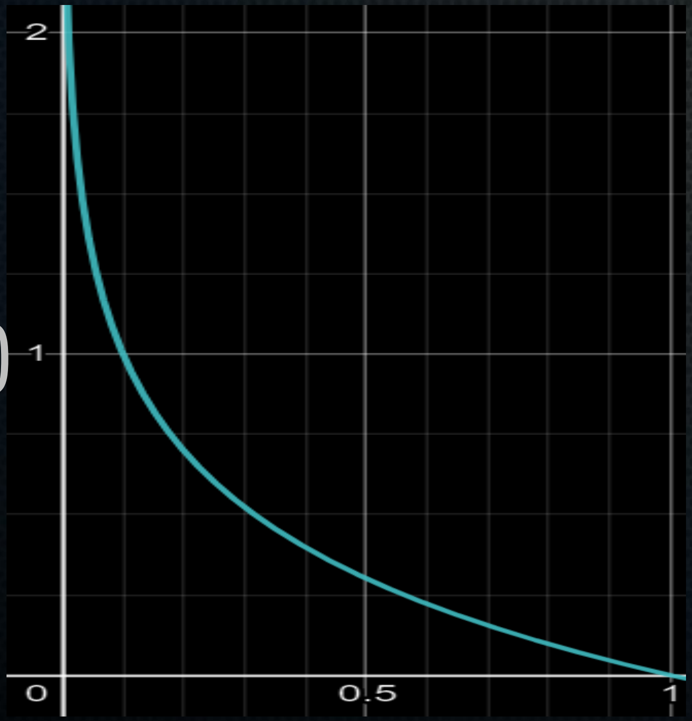

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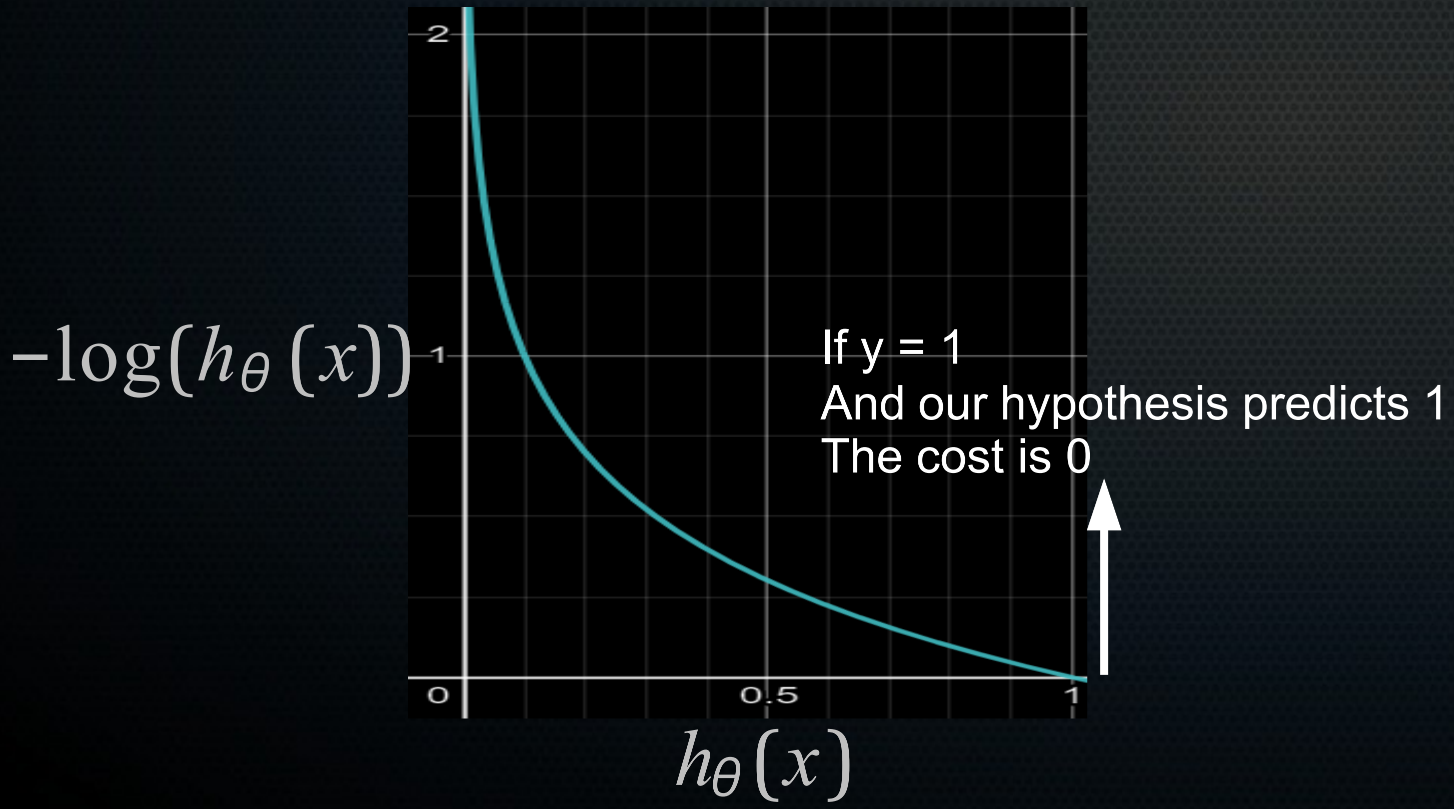

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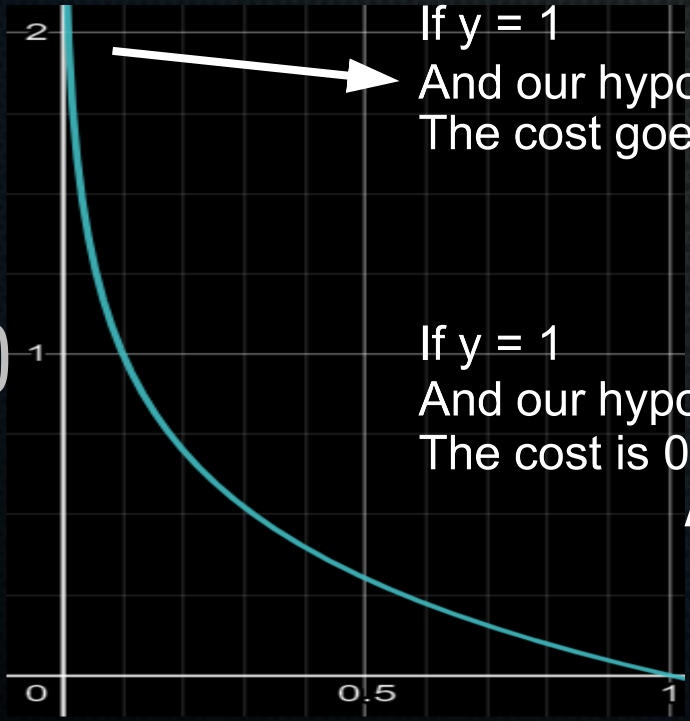

$h_\theta(x)$

If y = 1
And our hypothesis predicts 0
The cost goes to ∞

If y = 1
And our hypothesis predicts 1
The cost is 0

What does this function look like?

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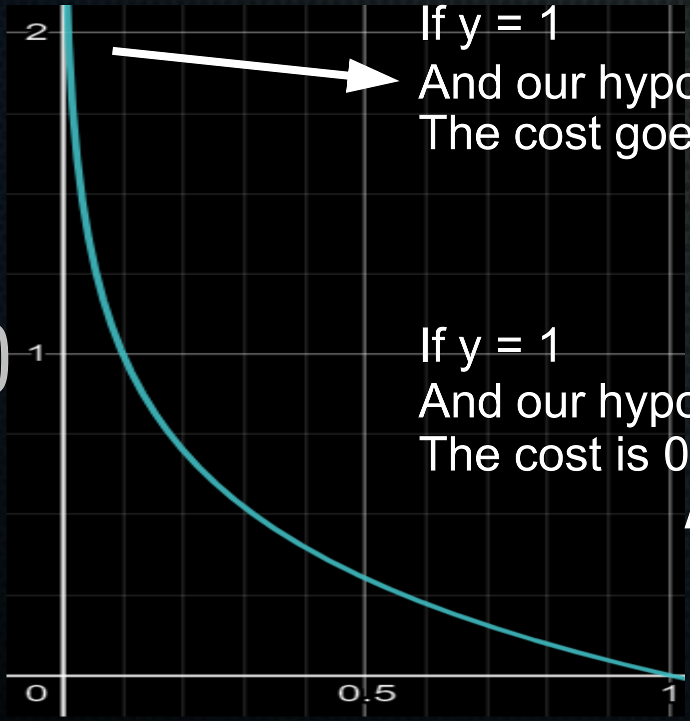

$h_\theta(x)$

If y = 1
And our hypothesis predicts 0
The cost goes to ∞

If we had used MSE

$$(0-1)^2 = 1$$

Penalised far less!

If y = 1
And our hypothesis predicts 1
The cost is 0

What does this function look like?

$$\text{Cost}(x) = \begin{cases} -\log(h_\theta(x)) \text{ if } y = 1 \\ \boxed{-\log(1 - h_\theta(x)) \text{ if } y = 0} \end{cases}$$

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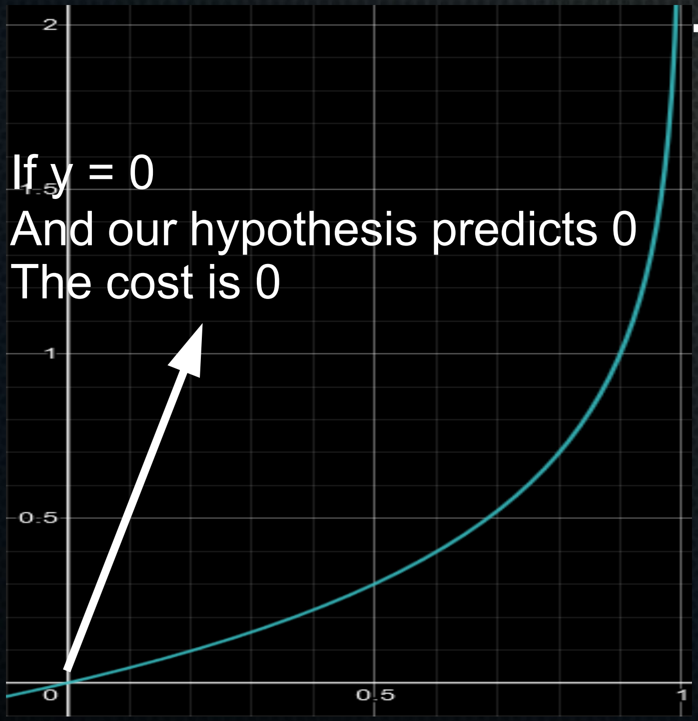

If y = 0
And our hypothesis predicts 0
The cost is 0

$h_\theta(x)$

If y = 0
And our hypothesis predicts 1
The cost goes to ∞

Simplified notation

$$\text{Cost}(x) = \begin{cases} -\log(h_\theta(x)) \text{ if } y=1 \\ -\log(1-h_\theta(x)) \text{ if } y=0 \end{cases}$$

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}(x^i)$$

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$y = 1$

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$$\boxed{-\log(h_\theta(x))}$$

Putting it all together

$$\mathrm{Cost}(x) = -\,y \cdot \log\left(h_\theta(x)\right) - (1-y) \cdot \log\left(1-h_\theta(x)\right) \qquad J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \mathrm{Cost}(x^i)$$

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} -\,y^{(i)} \cdot \log\left(h_\theta(x^{(i)})\right) - (1-y^{(i)}) \cdot \log\left(1-h_\theta(x^{(i)})\right)$$

Putting it all together

$$\mathrm{Cost}(x) = -y \cdot \log(h_\theta(x)) - (1-y) \cdot \log(1-h_\theta(x)) \qquad J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \mathrm{Cost}(x^i)$$

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$$J(\theta) = \boxed{-} \frac{1}{m}\sum_{i=1}^{m} y^{(i)} \cdot \log(h_\theta(x^{(i)})) + (1-y^{(i)}) \cdot \log(1-h_\theta(x^{(i)}))$$

Optimising the cost function

- Same form as for linear regression (only hypothesis function differs!)

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} ((\boxed{h_\theta(x^{(i)})} - y^{(i)}) \cdot x_j^{(i)})$$

$$\theta_j := \theta_j - \frac{a}{m} \sum_{i=1}^{m} ((\boxed{h_\theta(x^{(i)})} - y^{(i)}) \cdot x_j^{(i)})$$

$$\boxed{h_\theta(x^{(i)}) = \frac{1}{1 + e^{-\theta^T * x}}}$$

Derivation link

Summary

- By using the sigmoid function as a transformation of normal regression and interpreting the output as a chance of being 0 or 1 we can do classification.
- Only the form of our hypothesis function is different
- Need a different cost function: should be smooth, and give logical values for large errors.

Break for practical