#### Course content: what I hope to teach you

- What is ML? Cost functions, gradient descent, generalisation, bias and variance.
- Week 1: low-level understanding: able to implement linear regression, logistic regression, neural networks, clustering and PCA yourself using numpy in Python.
- Week 2: modern ML library (scikit-learn) workflow (one day), + a hands-on project (~2 days). Written exam about lecture and practical concepts at the end.

#### Setup per day

- Morning/early afternoon:
  - Lectures of ~45-60 minutes, interspersed with (2) short practical(s).
- Rest of the day:
  - Somewhat longer afternoon practical
- Taken together:
  - Lecture
  - Short practical 1
  - Lecture
  - Short practical 2
  - Lecture
  - Afternoon practical



 This is a new course. So probably, you'll encounter difficulty spikes, things that don't make sense, or other things that are lacklustre.



- At the end of each practical I ask you to anonymously:
  - Rate how much you learned
  - Rate how difficult it was
  - Leave an extra comment to elaborate (optional)
- In this way, I can hopefully take things on board quickly and perhaps change practicals or lectures during the course, rather than only after!



You might wonder what's up with the coloured baubles I

blessed you with.



- You might wonder what's up with the coloured baubles I blessed you with.
- They're mood indicators for during the lecture:
  - Green: "I am positively brimming with enthusiasm to learn" and/or "I can follow this material well enough"
  - Yellow/Orange: "This is somewhat difficult" and/or "I feel my attention is slipping and I can't absorb the information so well anymore"
  - Red: "MAKE IT STOP! PLEASE, PLEASE MAKE IT STOP!!!"









- Put the bauble that matches your mood at the front of your table.
- I tend to make lectures a bit too long. In this way, I can notice that's happening and stop it, without you having to tell me to shut up. Win-win!







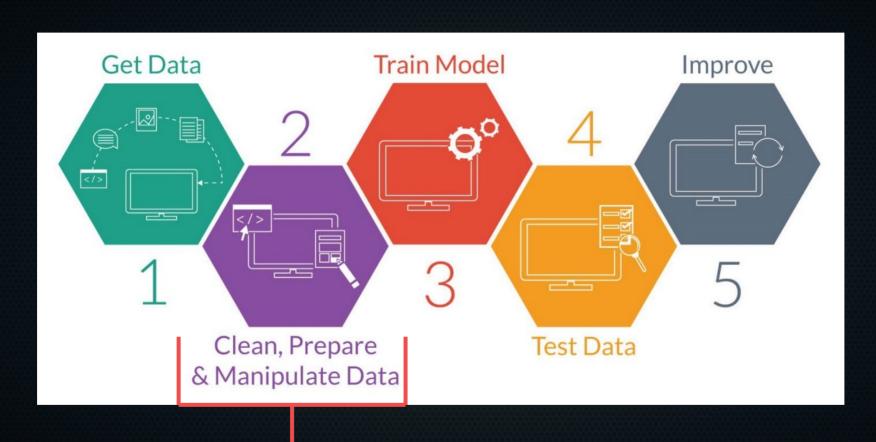


#### Questions

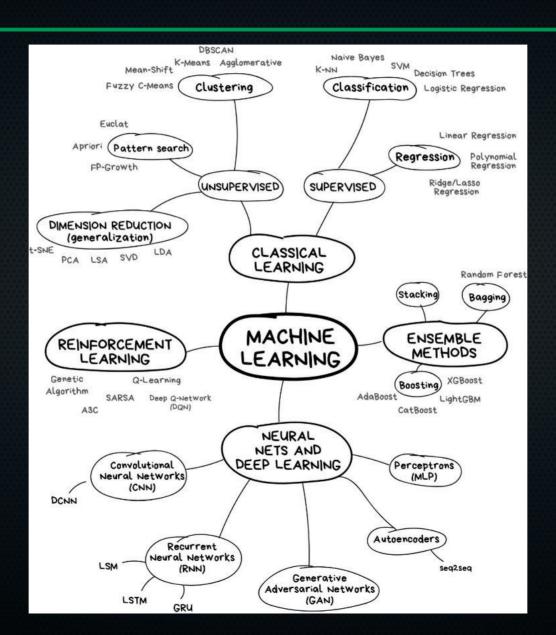
 Besides this, feel free to raise your hand and ask questions when something is unclear.

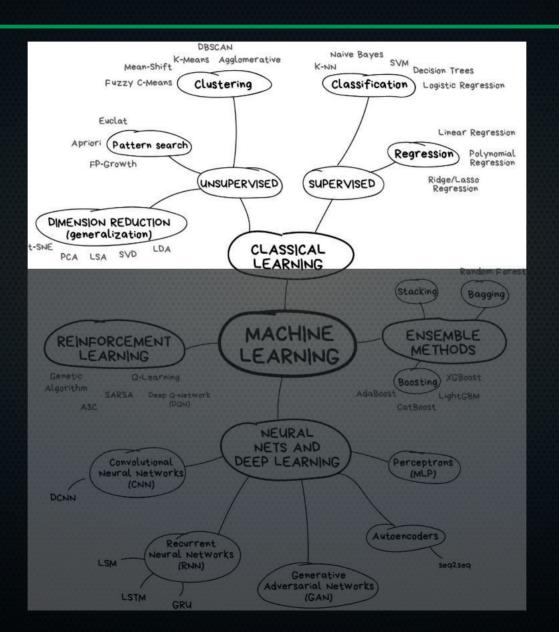
• If there's no hands raised right now then we'll dive right in!

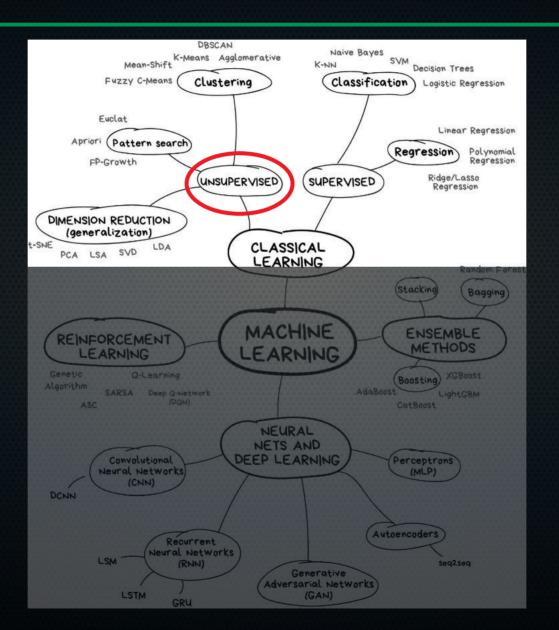
# The ugly truth about ML

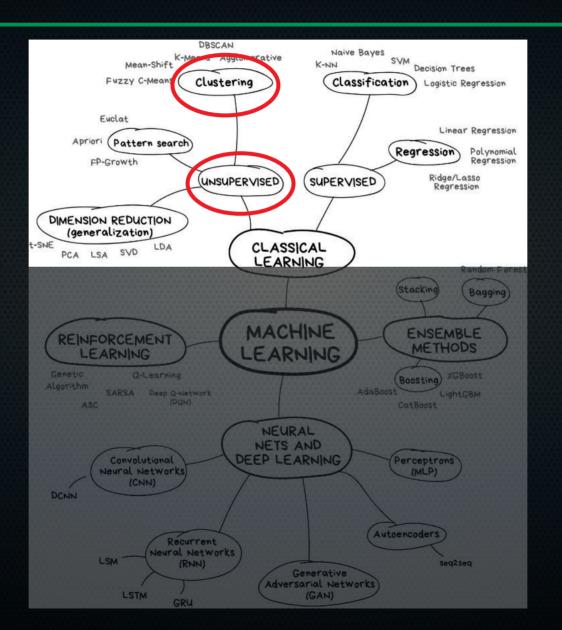


80% of your time

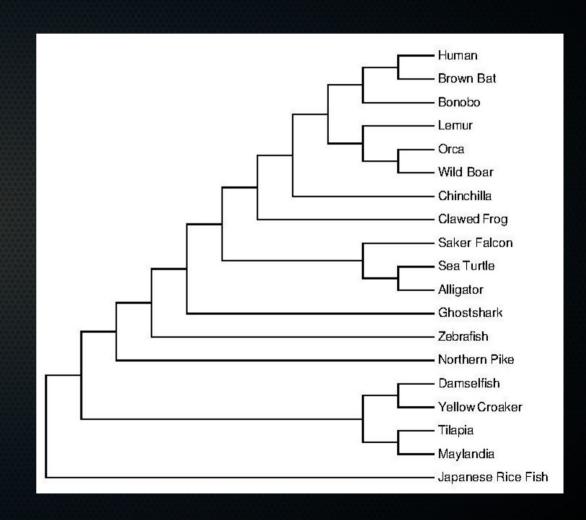




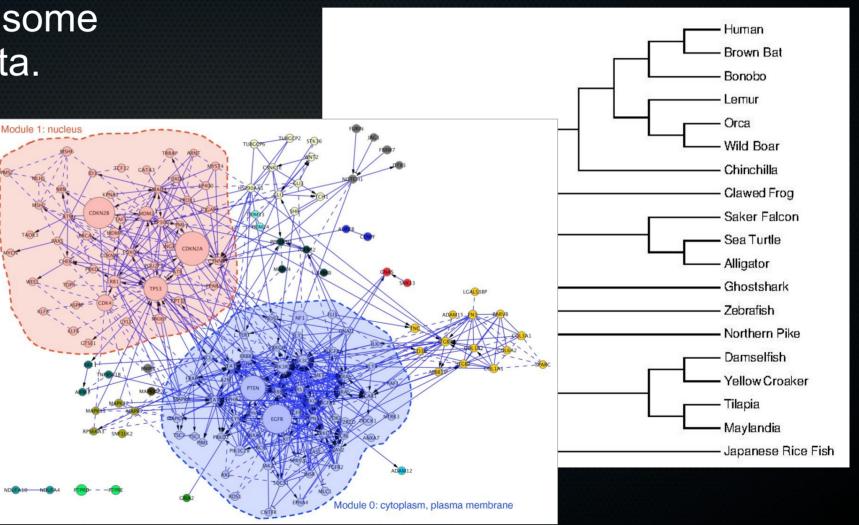


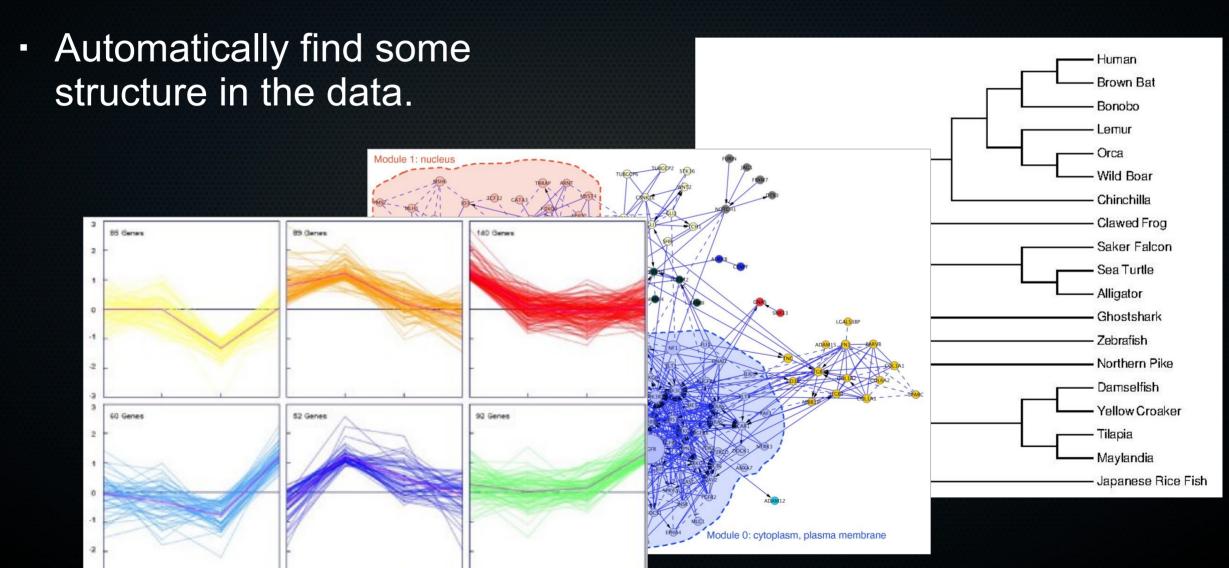


 Automatically find some structure in the data.

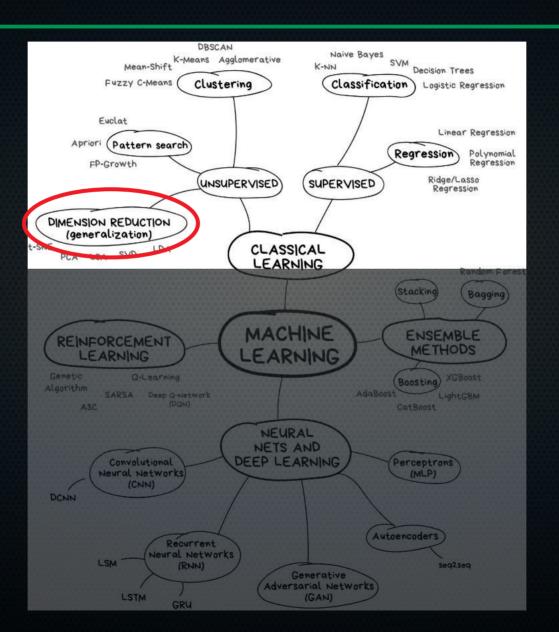


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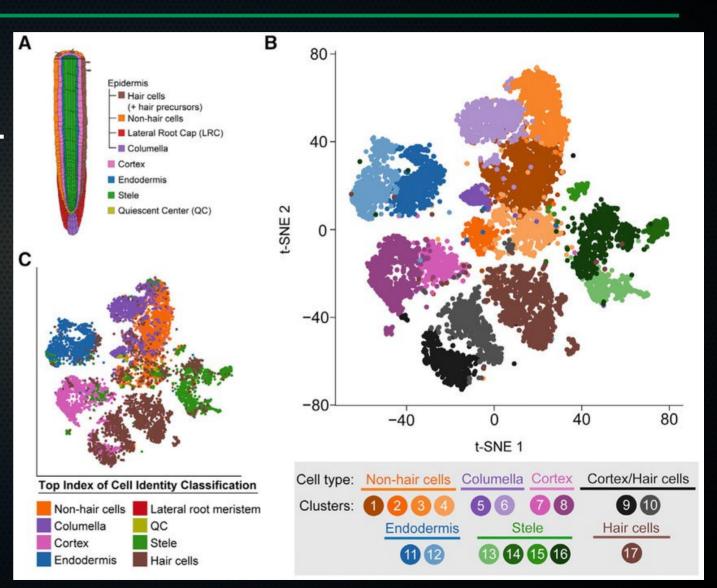


- No right or wrong:
  - Back-and-forth between different clustering algorithms, your knowledge, and the data.
  - You don't know correct clustering.



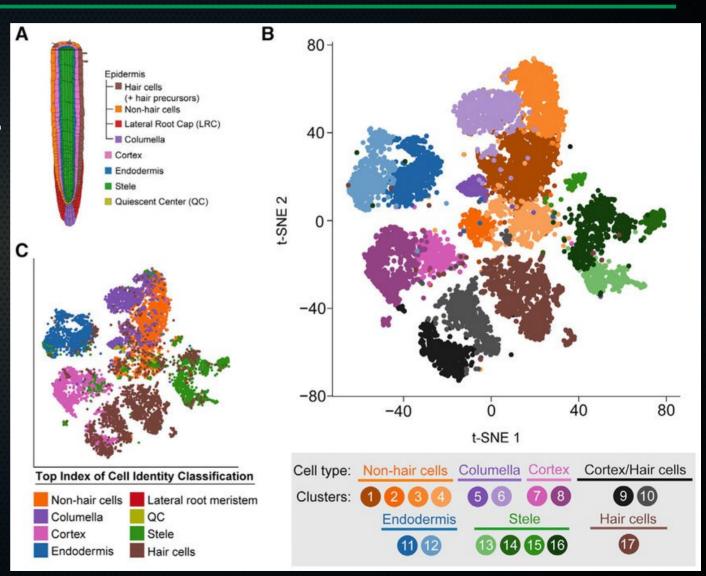
## Unsupervised learning: dimensionality reduction

- Single-cell RNAseq of 12,198 Arabidopsis root cells.
- How do they differ?



#### Unsupervised learning: dimensionality reduction

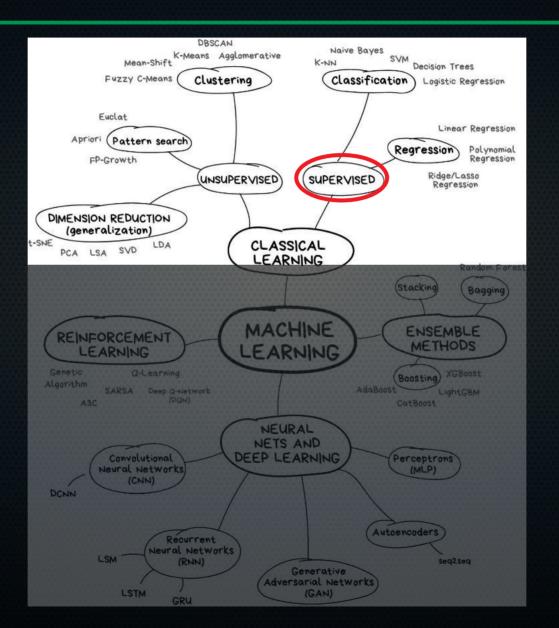
- Single-cell RNAseq of 12,198 Arabidopsis root cells.
- How do they differ?
- Visualise differences in all RNAs between all these cells in 2 dimensions.
- Used in conjunction with clustering (colours)



#### Unsupervised learning: dimensionality reduction

#### Used for:

- Visualisation (our visual systems cannot deal with > 3D)
- Compressing data (capture 90% of the variation with much less data, say)
- AFMAKEN

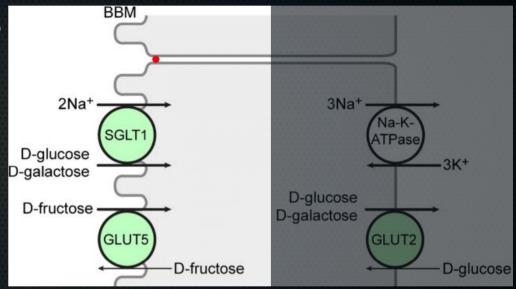


## Supervised learning

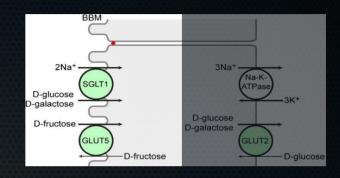
 Given known examples, automatically find a function to map new examples.

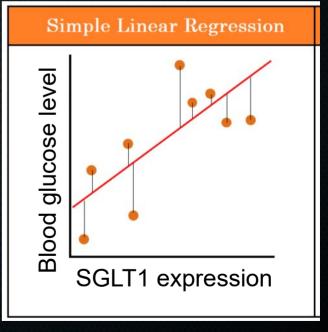
 Given known examples, automatically find a function to map new examples.

Real-valued outputs.

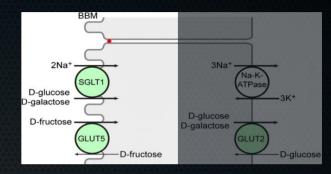


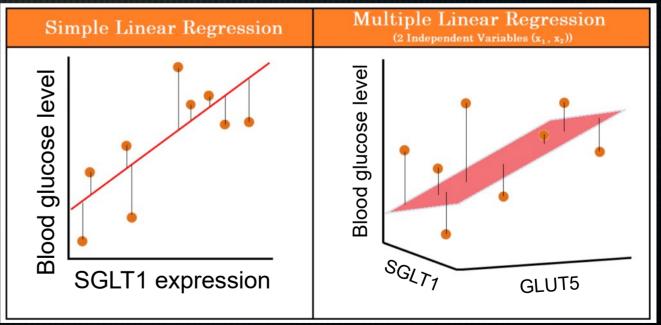
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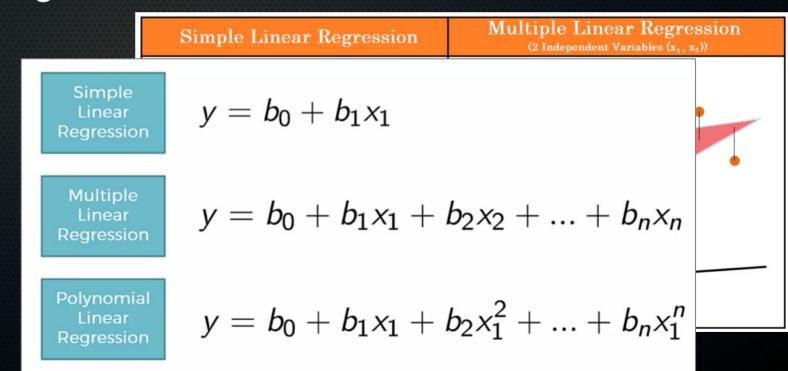


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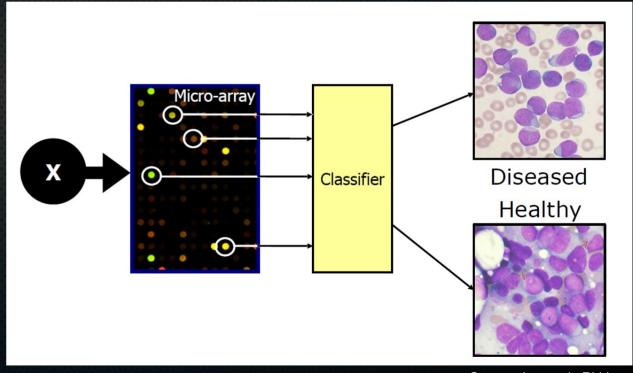




- Given known examples, automatically find a function to map new examples.
- Real-valued outputs: regression.

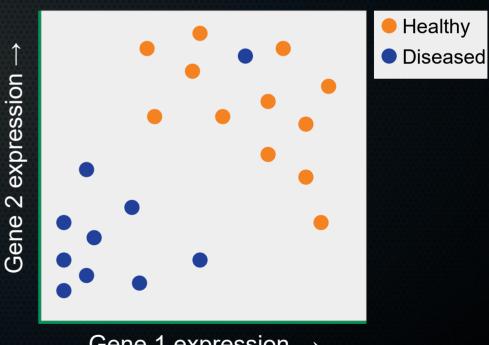


- Given known examples, automatically find a function to map new examples.
- Discrete outputs.



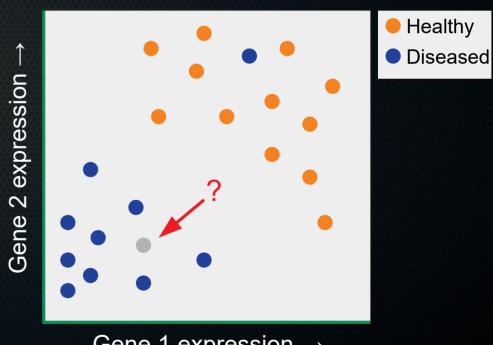
Source: Jeroen de Ridder

- Given known examples, automatically find a function to map new examples.
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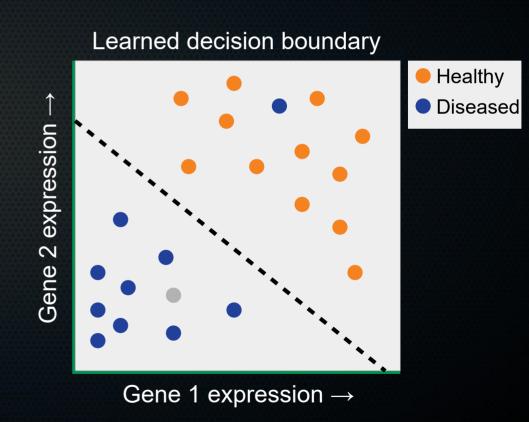


Gene 1 expression →

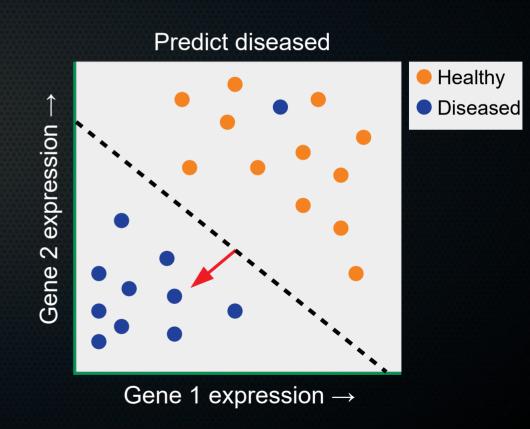
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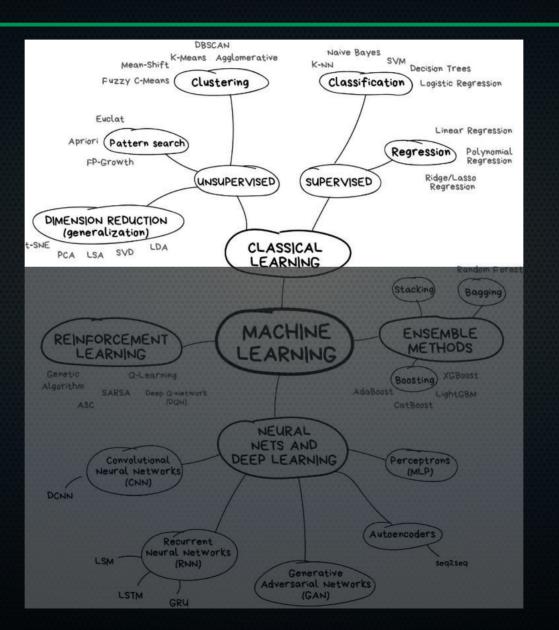


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#### Summary

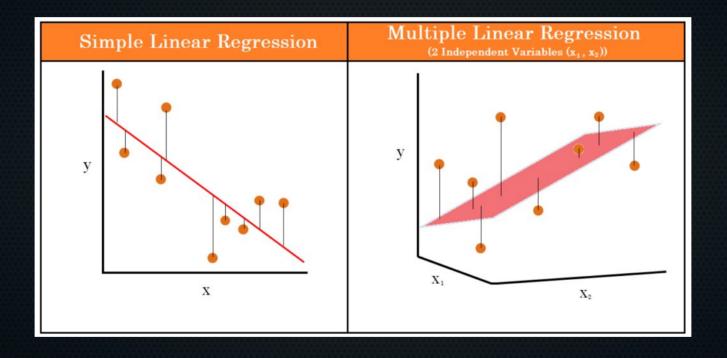
#### Unsupervised:

- Find some structure in your data (clusters, projection into lowerdimensional space that captures much of variance)
- Don't know the "correct" structure (no labels)

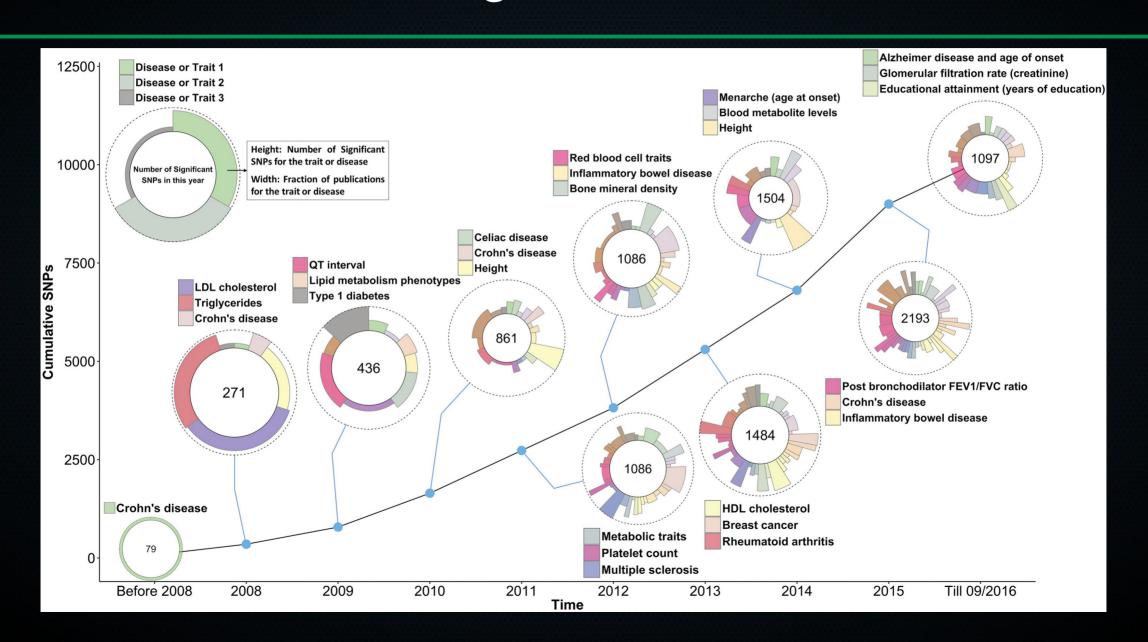
#### Supervised:

Automatically learn a function that maps features (e.g. gene expression) to a real-valued output (regression, e.g. blood glucose level) or discrete classes/labels (classification, e.g. healthy/diseased) using training data for which you know these outcomes.

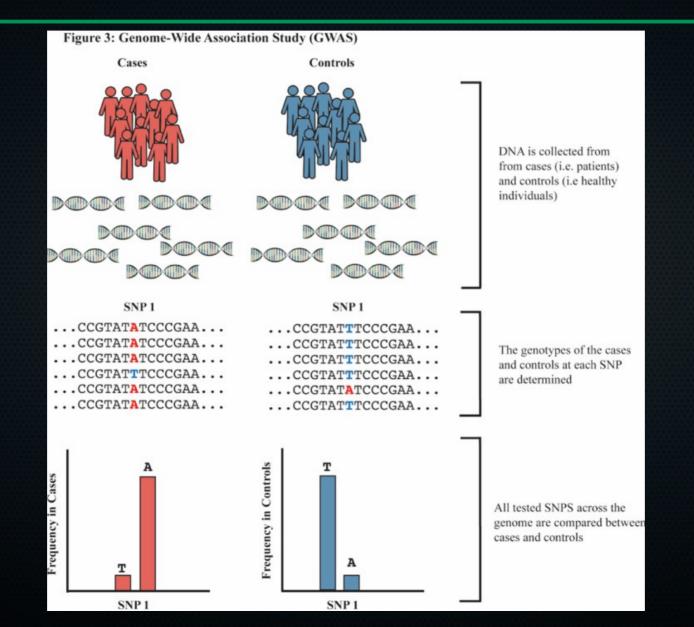
## Linear regression



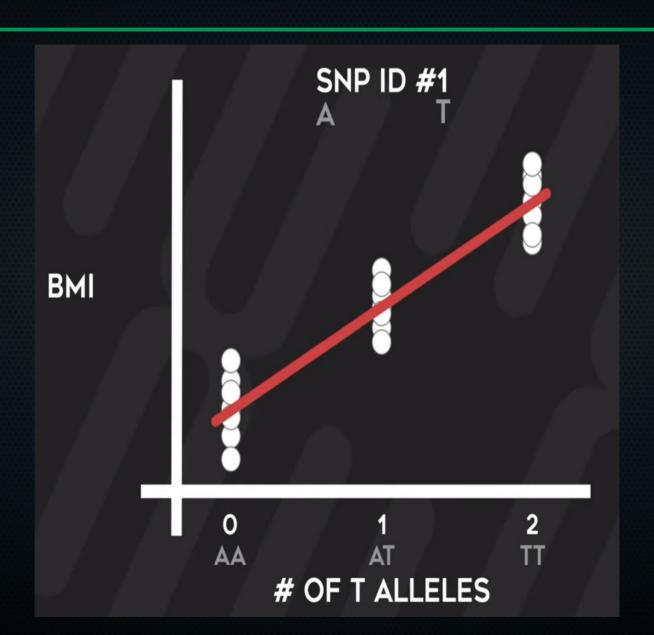
## Linear regression: GWAS



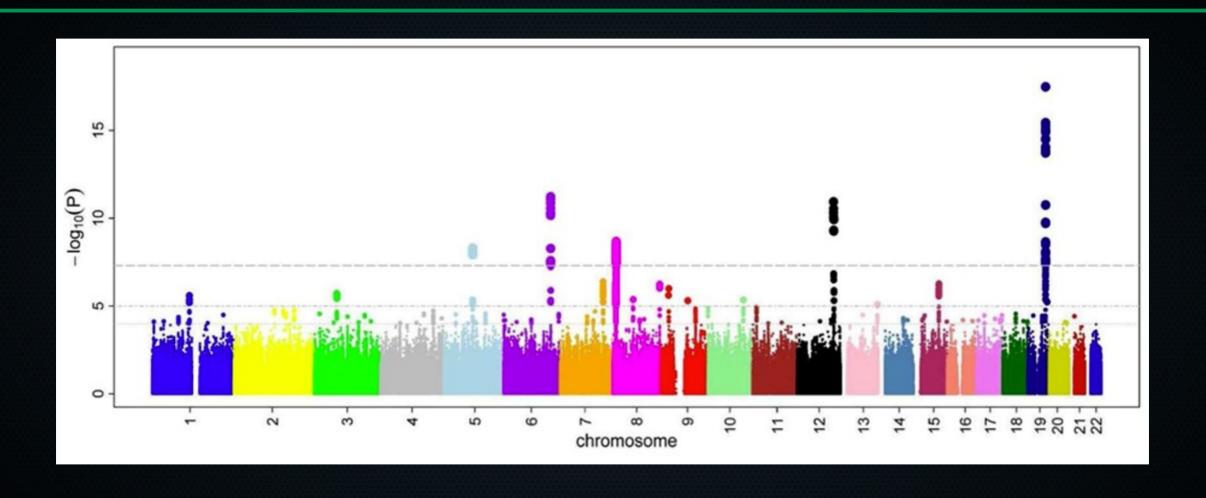
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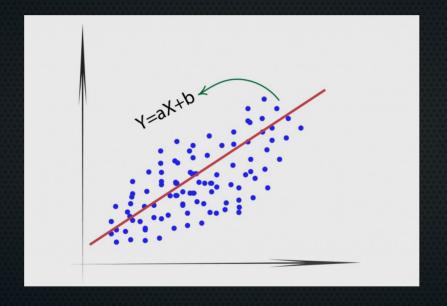


### Linear regression: GWAS

- Connect SNPs to nearby genes (non-trivial!)
- Yielded huge advances in our knowledge on many complex diseases over the past ~15 years.

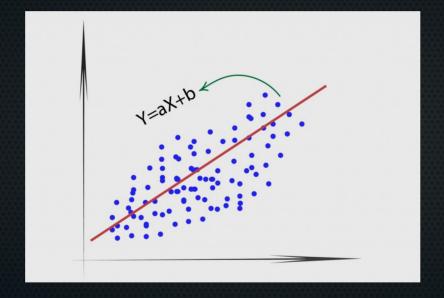
# Univariate linear regression

$$y = ax + b$$



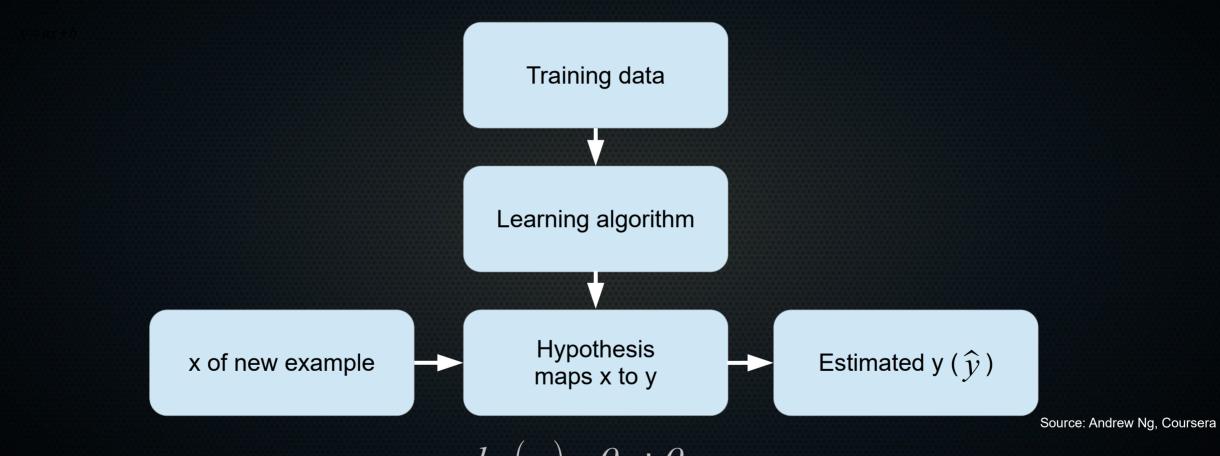
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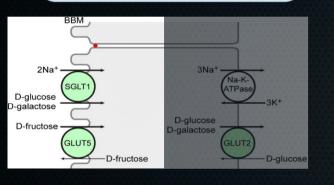
$$y = \theta_0 + \theta_1 x$$

### Process



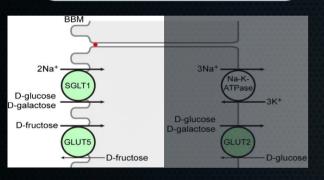
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

#### Training data



Sample #	SGLT1 expression level (arbitrary units relative to housekeeping gene)	Blood glucose level (mg/dL)
1	3	80
2	8	130
3	12	170
4	2	89

Training data

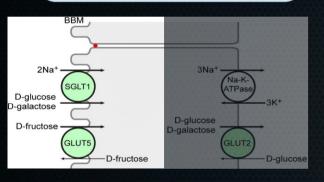


m = # of training examples

m

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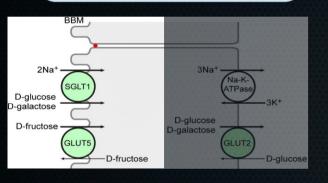
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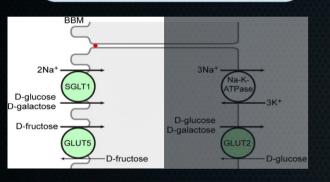
Training data



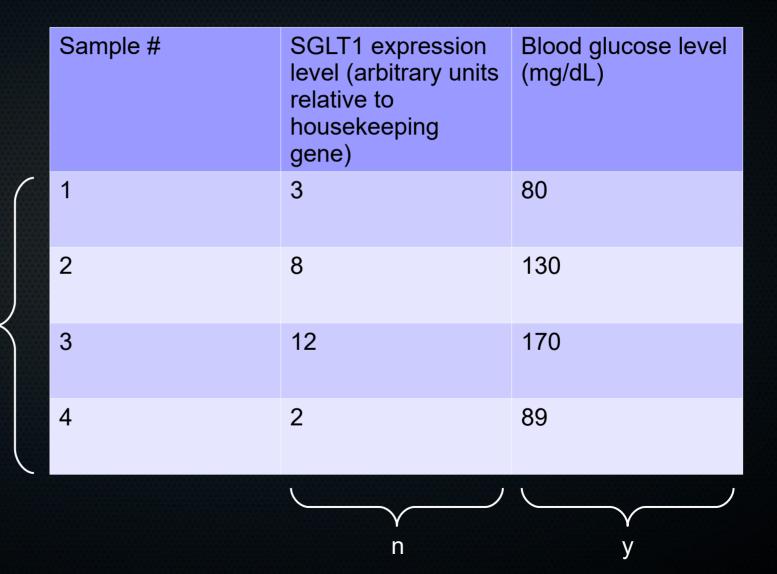
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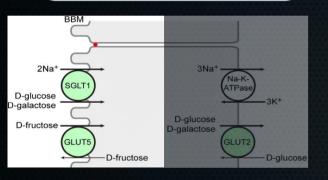
Training data



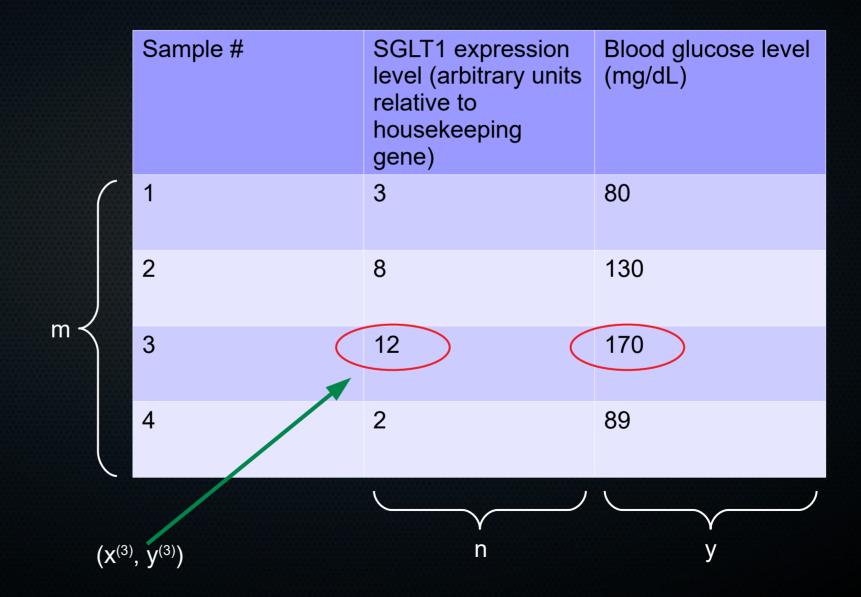
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Training data



m = # of training examples n = # of features/variables y = output variable/target variable or label (classification)  $(x^{(i)}, y^{(i)})$  = i-th training example



### Cost function and gradient descent

- How to learn theta's from data?
- Two parts
  - How wrong are we for given parameters?
  - How do we update our parameters, given how wrong we are?

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

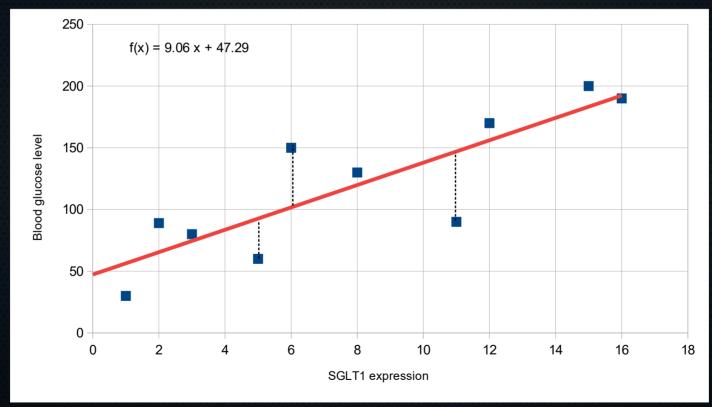
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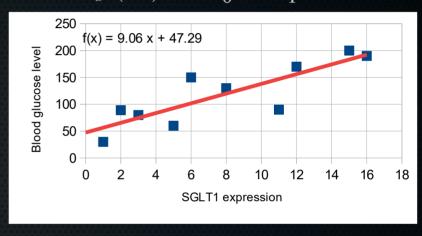
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$



- How wrong are we for given parameters?
- Cost function:

$$J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

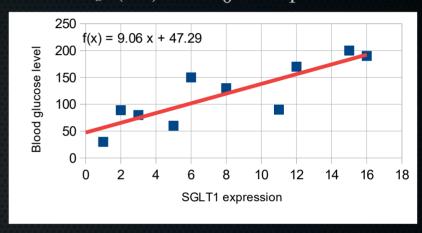


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$$J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

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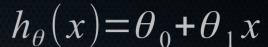


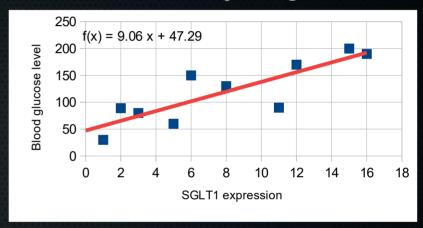
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$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$





How wrong are we for given parameters?

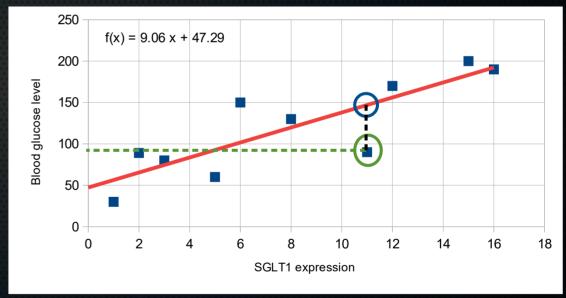
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Cost function:

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$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - (y^{(i)})^2$$



### Cost function conclusion

If we want to be as correct as possible with our prediction, want to minimise:  $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$ 

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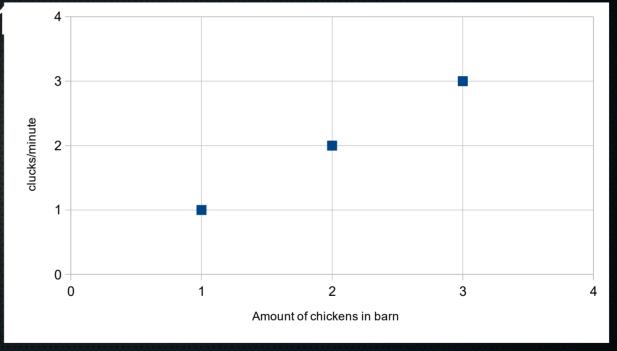
Simplified example: Theta0 = 0:

$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_1 \cdot x^{(i)} - y^{(i)})^2$$

#### Cost function conclusion illustration

Let's say theta0 = 0 (so the intercept is 0). What is J(theta1)

for different values of theta1





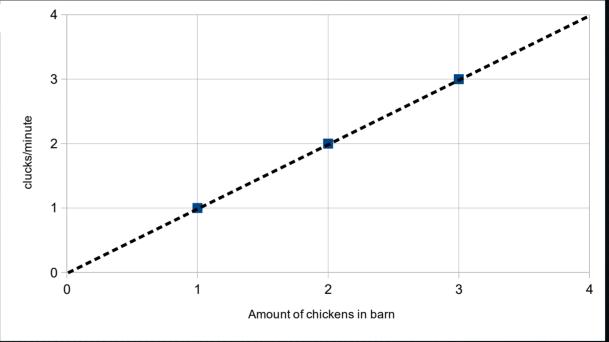
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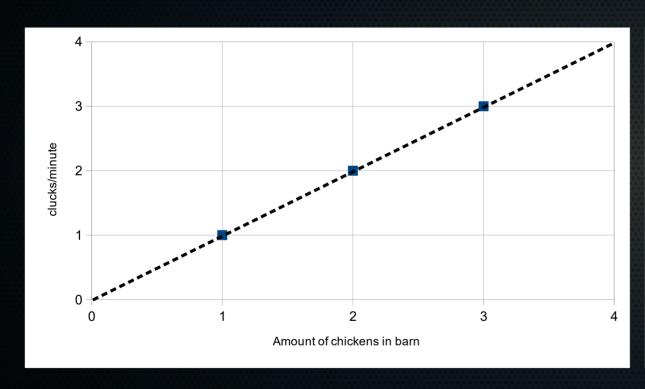
Theta1 = 1

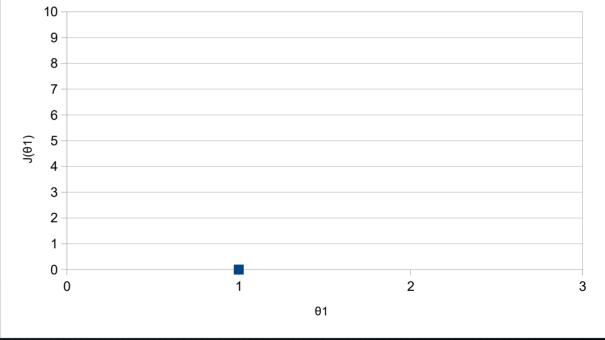
$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{3} (\theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$J(\theta_1)=0$$







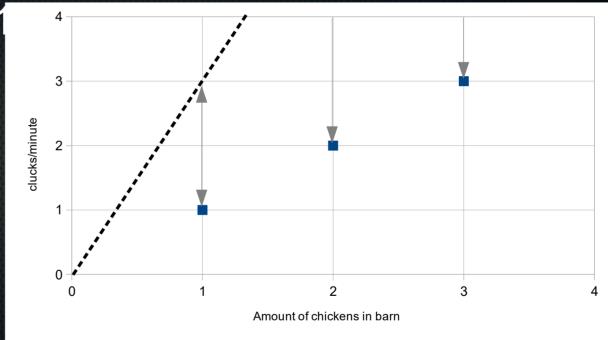


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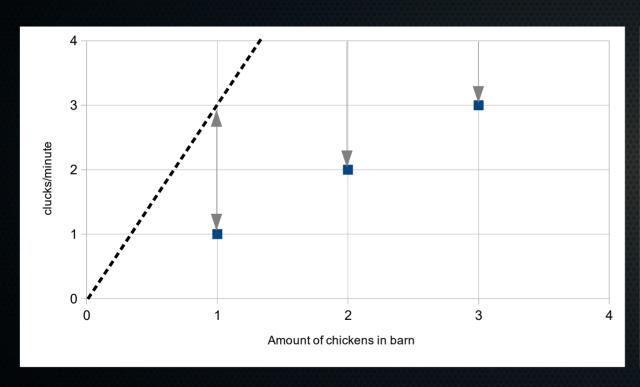
Theta1 = 3

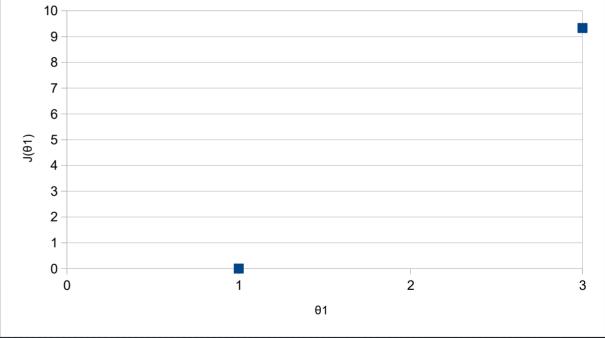
$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{3} (\theta_1 \cdot x^{(i)} - y^{(i)})^2$$



$$J(\theta_1) = \frac{1}{2 \cdot 3} \cdot ((3-1)^2 + (6-2)^2 + (9-3)^2) = 56/6 \approx 9.3$$





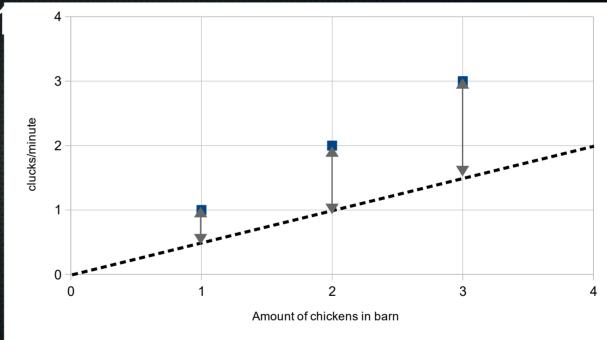


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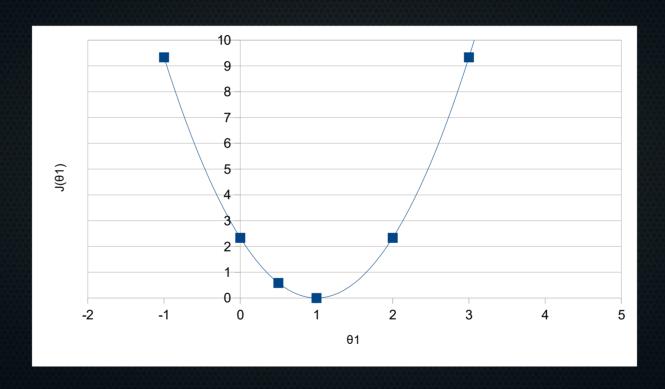
- Theta1 = 0.5

$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{3} (\theta_1 \cdot x^{(i)} - y^{(i)})^2$$



$$J(\theta_1) = \frac{1}{2 \cdot 3} \cdot ((0.5 - 1)^2 + (1 - 2)^2 + (1.5 - 3)^2) = 3.5/6 \approx 0.6$$

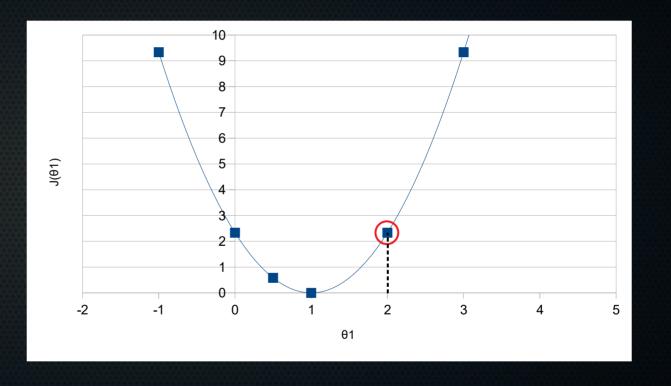




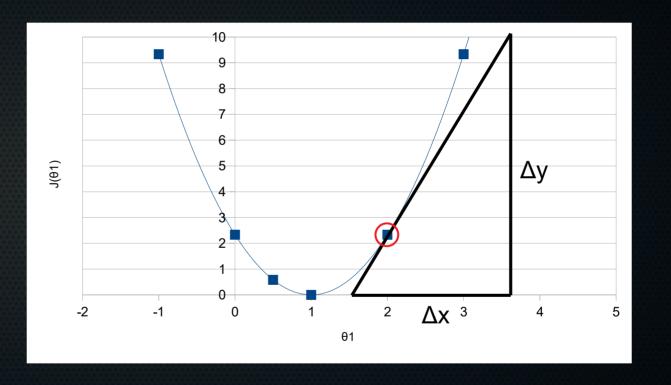
### Cost function and gradient descent

- How to learn theta's from data?
- Two parts
  - How wrong are we for given parameters?
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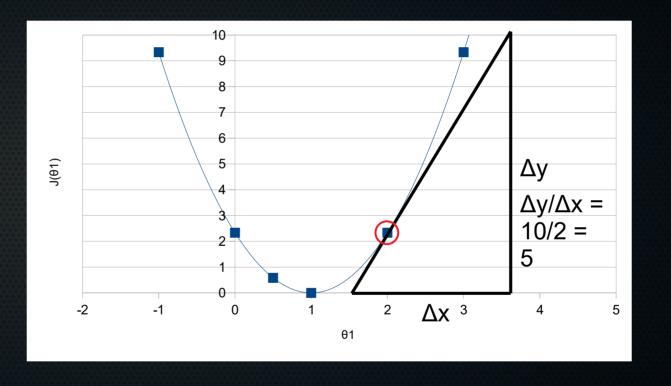
- Want to minimise
- Where to go?



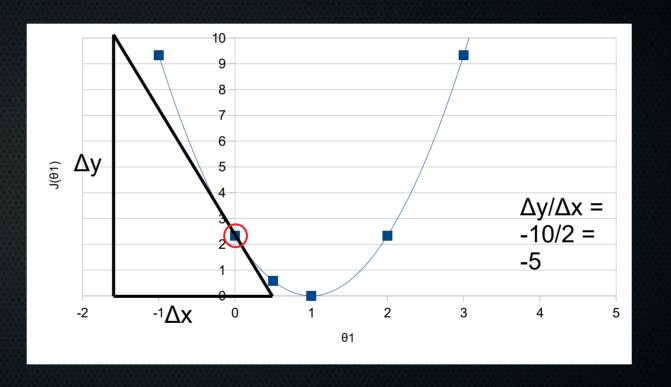
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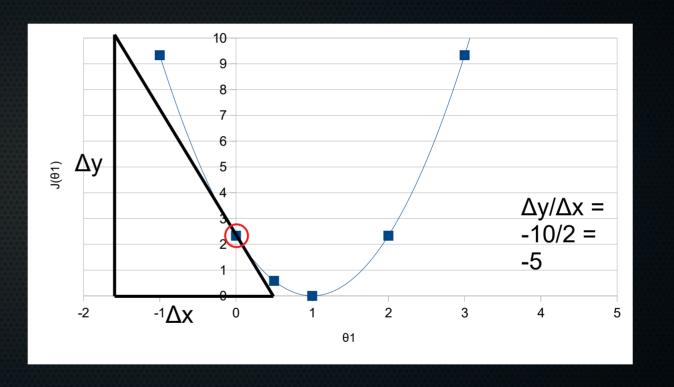


- Want to minimise
- Where to go?



- Want to minimise
- Where to go?
- Change current theta1 as follows:

$$\theta_1 = \theta_1 - \alpha \cdot \frac{d}{d\theta_1} J(\theta_1)$$



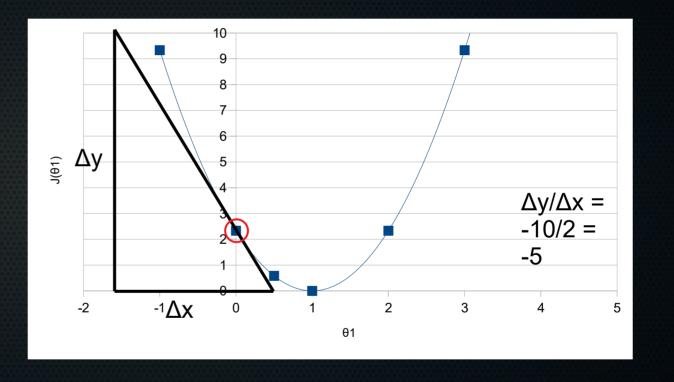
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$$\theta_1 = \theta_1 - \alpha \cdot \frac{d}{d\theta_1} J(\theta_1)$$

$$\alpha = 0.2$$

$$\theta_1 = 0 - 0.2 \cdot -5$$

$$\theta_1 = 1$$



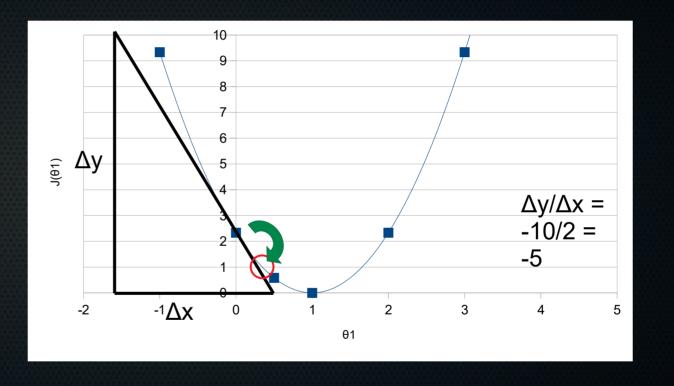
- Want to minimise
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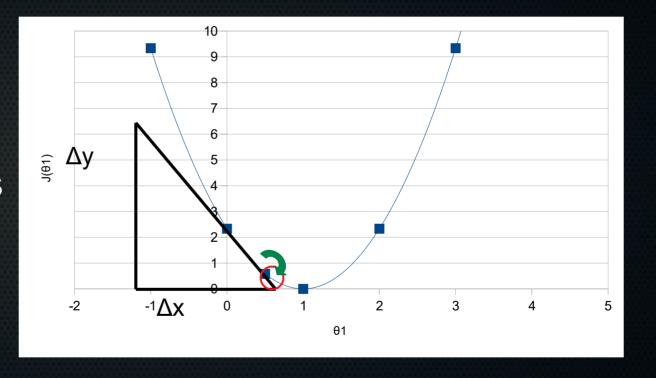
$$\alpha = 0.2$$

$$\theta_1 = 0 - 0.2 \cdot -5$$

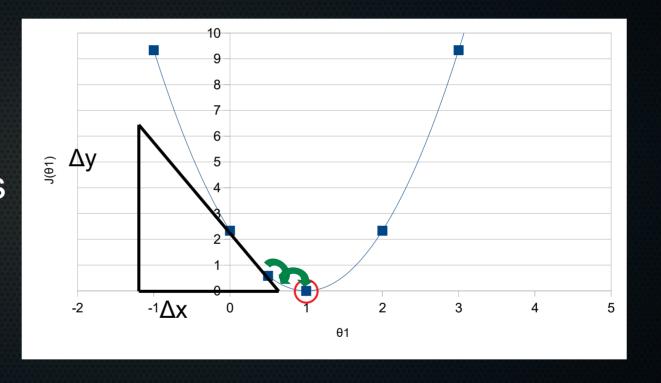
$$\theta_1 = 1$$



- Want to minimise
- Where to go?
- Change current theta1
- Note: gradient becomes smaller closer to optimum, so can use fixed value for α



- Want to minimise
- Where to go?
- Change current theta1
- Note: gradient becomes smaller closer to optimum, so can use fixed value for α



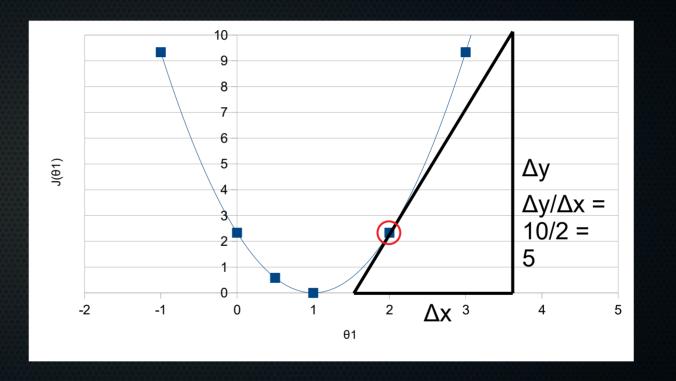
 Works also from other direction.

$$\theta_1 = \theta_1 - \alpha \cdot \frac{d}{d\theta_1} J(\theta_1)$$

$$\alpha = 0.2$$

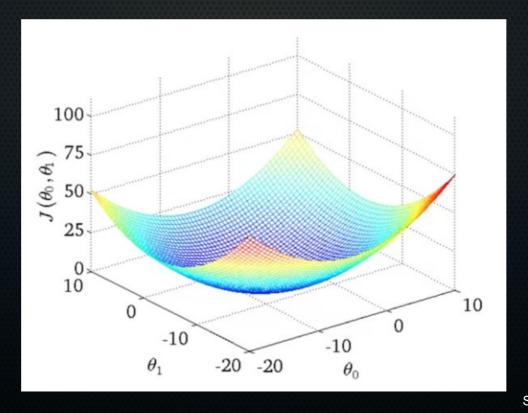
$$\theta_1 = 2 - 0.2 \cdot 5$$

$$\theta_1 = 1$$



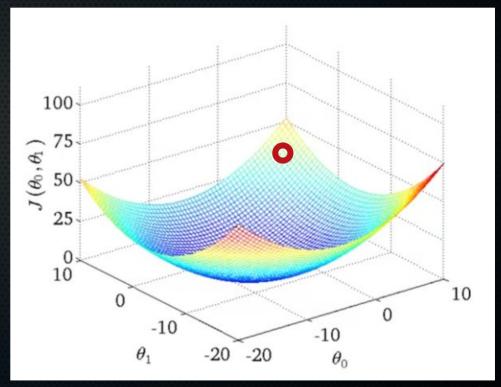
 Iteratively descend down the gradient of the cost function until convergence → optimal parameters!

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- In reality: not one-dimensional:



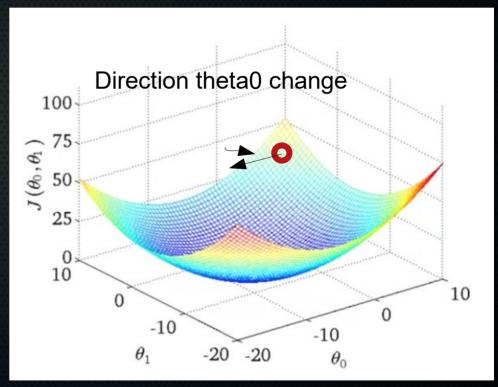
 Iteratively descend down the gradient of the cost function until convergence → optimal parameters!

- In reality: not one-dimensional.
   Want to fit intercept and slope.
- Use partial derivatives instead:



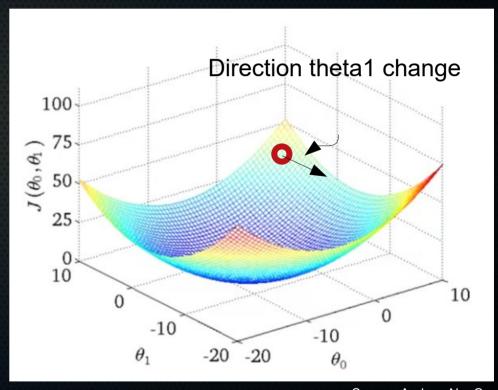
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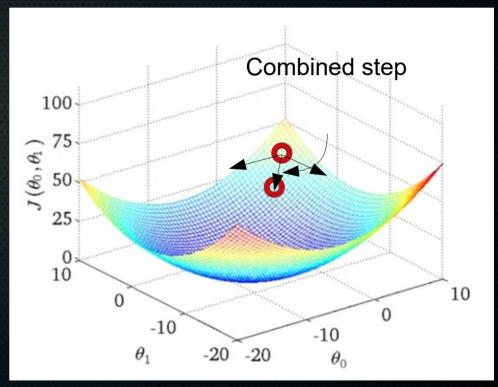
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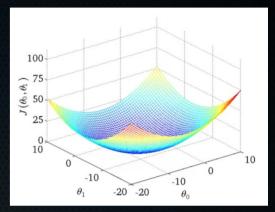
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#### Partial derivatives:

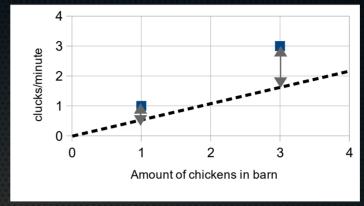
$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

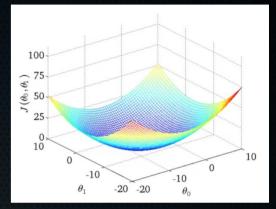


#### Partial derivatives:

m=2

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$





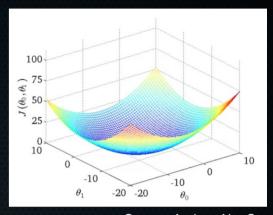
$$J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} ((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)})^2 + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)})^2)$$

$$f(g(x)) \qquad \frac{dy}{dx} = f'(g(x)) \times g'(x)$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

$$J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} ((\underline{\theta_0} + \theta_1 \cdot x^{(1)} - y^{(1)})^2 + (\underline{\theta_0} + \theta_1 \cdot x^{(2)} - y^{(2)})^2)$$



Source: Andrew Ng, Coursera

$$f(\underline{g}(x))$$

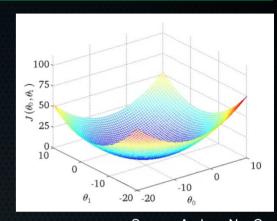
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$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} (2(\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)}) * 1$$
$$+ 2(\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)}) * 1)$$



Source: Andrew Ng, Courser

$$f(\underline{g(x)})$$

$$\frac{dy}{dx} = \underline{f'(g(x))} \times g'(x)$$

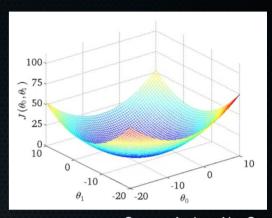
$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

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Source: Andrew Ng, Courser

$$f(\underline{g(x)})$$

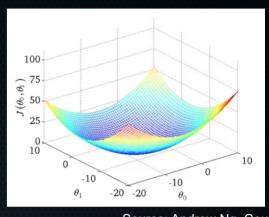
$$\frac{dy}{dx} = \underline{f'(g(x))} \times \underline{g'(x)}$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

$$J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} ((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)})^2 + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)})^2)$$

$$g'(x) = \frac{\partial}{\partial \theta_0} (1 \cdot \theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)}) = 1$$



Source: Andrew Ng, Coursera

$$f(\underline{g(x)})$$

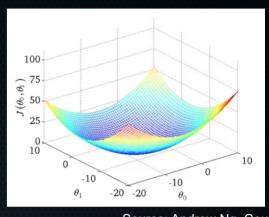
$$\frac{dy}{dx} = \underline{f'(g(x))} \times \underline{g'(x)}$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

$$J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} ((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)})^2 + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)})^2)$$

$$f'(g(x)) = \frac{\partial}{\partial \theta_0} (g(x))^2 = 2 \cdot g(x)$$



Source: Andrew Ng, Coursera

$$f(\underline{g(x)})$$

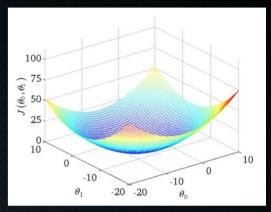
$$\frac{dy}{dx} = \underline{f'(g(x))} \times \underline{g'(x)}$$

$$J(\theta_{0}, \theta_{1}) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_{0} + \theta_{1} \cdot x^{(i)} - y^{(i)})^{2}$$

$$m = 2$$

$$\frac{\partial}{\partial \theta_{0}} J(\theta_{0}, \theta_{1}) = \frac{1}{2 \cdot 2} (2(\theta_{0} + \theta_{1} \cdot x^{(1)} - y^{(1)}) * 1$$

$$+2(\theta_{0} + \theta_{1} \cdot x^{(2)} - y^{(2)}) * 1)$$



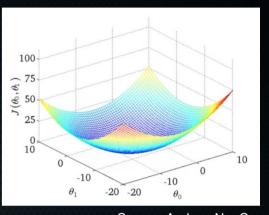
Source: Andrew Ng, Coursera

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Source: Andrew Ng, Coursera

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{n} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

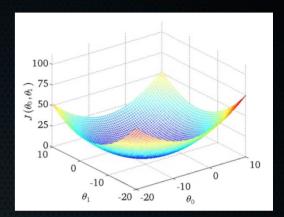
$$m = 2$$

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} \left( 2 \left( (\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)}) * 1 + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)}) * 1 \right) \right)$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{n} (\theta_0 + \theta_1 \cdot x^{i} - y^{i})$$

$$m = 2$$

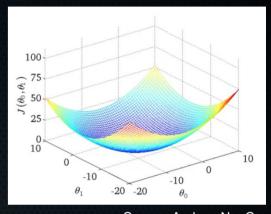


$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} (2((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)}) * 1 + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)}) * 1))$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{2} ((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)}) + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)}))$$



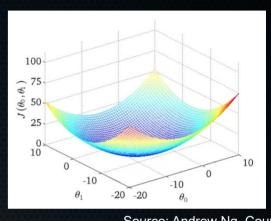
Source: Andrew Ng, Coursera

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

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$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m \left( \theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)} \right)$$



Source: Andrew Ng, Coursera

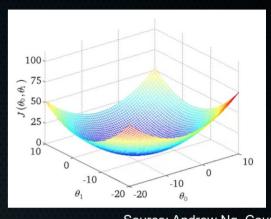
#### Partial derivatives:

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{2} ((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)}) + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)}))$$

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m \left( \theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)} \right) = \frac{1}{m} \sum_{i=1}^m \left( h_\theta(x^{(i)}) - y^{(i)} \right)$$



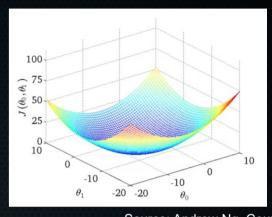
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$m=2$$

$$J(\theta_0, \theta_1) = \frac{1}{2 \cdot 2} ((\theta_0 + \theta_1 \cdot x^{(1)} - y^{(1)})^2 + (\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)})^2)$$

$$\frac{\partial}{\partial \theta_{1}} J(\theta_{0}, \theta_{1}) = \frac{1}{2 \cdot 2} (2(\theta_{0} + \theta_{1} \cdot x^{(1)} - y^{(1)}) * x^{(1)} + 2(\theta_{0} + \theta_{1} \cdot x^{(2)} - y^{(2)}) * x^{(2)})$$

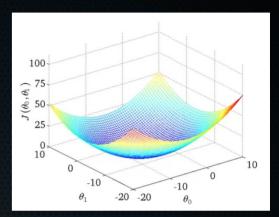


Source: Andrew Ng, Courser

$$f(g(x))$$
 
$$\frac{dy}{dx} = f'(g(x)) \times \underline{g'(x)}$$

Partial derivative theta1:

$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m \left( \left( h_{\theta}(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)} \right)$$



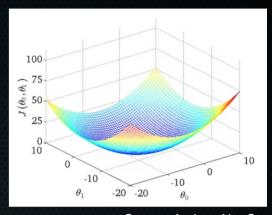
# Cost function and gradient descent

#### Cost function:

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x) - y^{(i)})^2$$

Partial derivatives for gradient descent:

$$\begin{split} &\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m \left( h_{\theta}(x^{(i)}) - y^{(i)} \right) \\ &\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m \left( \left( h_{\theta}(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)} \right) \end{split}$$



$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

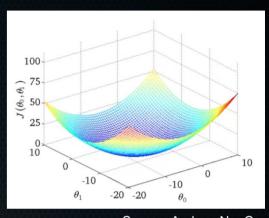
# Cost function and gradient descent

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$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x) - y^{(i)})^2$$

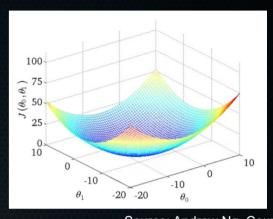
Gradient descent update:

$$\begin{split} &\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^m \left( h_\theta(x^{(i)}) - y^{(i)} \right) \\ &\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \theta_1 - \frac{\alpha}{m} \sum_{i=1}^m \left( \left( h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)} \right) \end{split}$$



$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

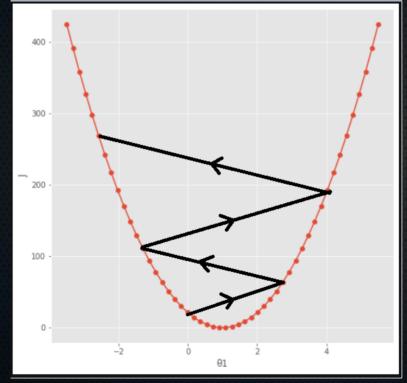
Learning rate, so-called hyperparameter.

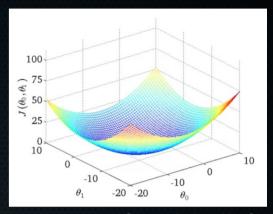


Source: Andrew Ng, Coursera

$$\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^m \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)$$

- Learning rate, so-called hyperparameter.
- Too high:



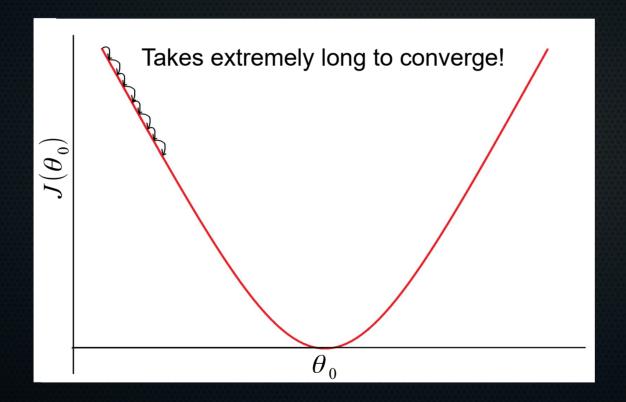


Source: Andrew Ng, Coursera

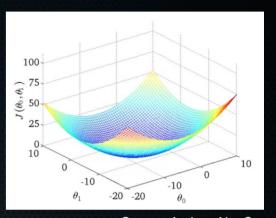
Source: https://towardsdatascience.com/univariate-linear-regression-theory-and-practice-99329845e85d

$$\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^m \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)$$

- Learning rate, so-called hyperparameter.
- Too low:

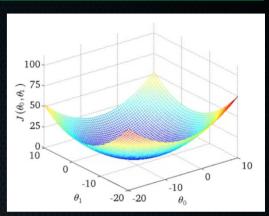


$$\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^m \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)$$



Source: Andrew Ng, Coursera

- Learning rate, so-called hyperparameter.
- Will discuss later how we pick it!



### Summary

- Defined a cost function for linear regression
- Showed how gradient descent can be used to minimise this cost function by changing the parameters
- Calculated partial derivatives for use with gradient descent
- Encountered our first hyperparameter, α, which governs the size of update steps