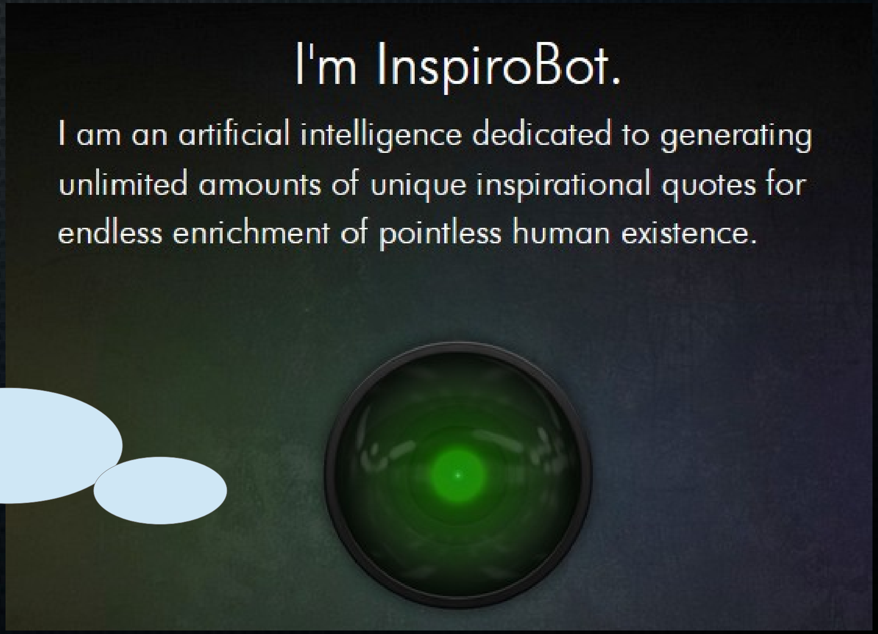
Daily Inspiration



Today

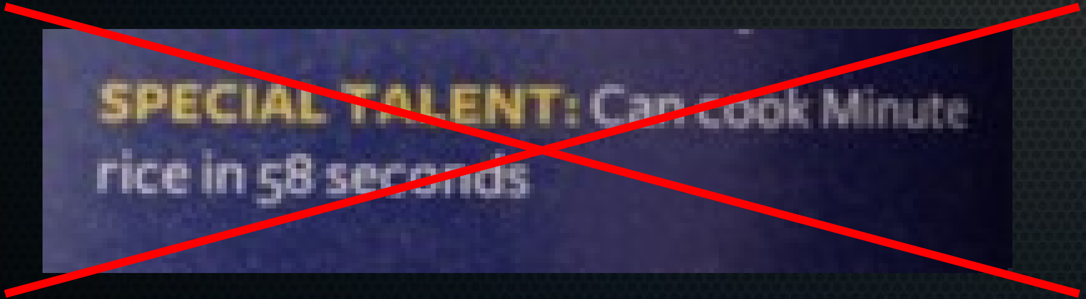
- Intro
- Linear regression, gradient descent
- Bias and variance, cross-validation, learning curves
- Linear algebra primer

Who am I?

- Some random guy off the streets
- Studied Biology, then Molecular and Cellular Life Sciences with Bioinformatics profile, doing mainly ML. Homegrown at UU.

Who am I?

- Some random guy off the streets
- Studied Biology, then Molecular and Cellular Life Sciences with Bioinformatics profile, doing mainly ML. Homegrown at UU.
- Hidden talent:



Can sing Tom Lehrer's Elements Song (used to, anyway)

- I can also tie my own shoes

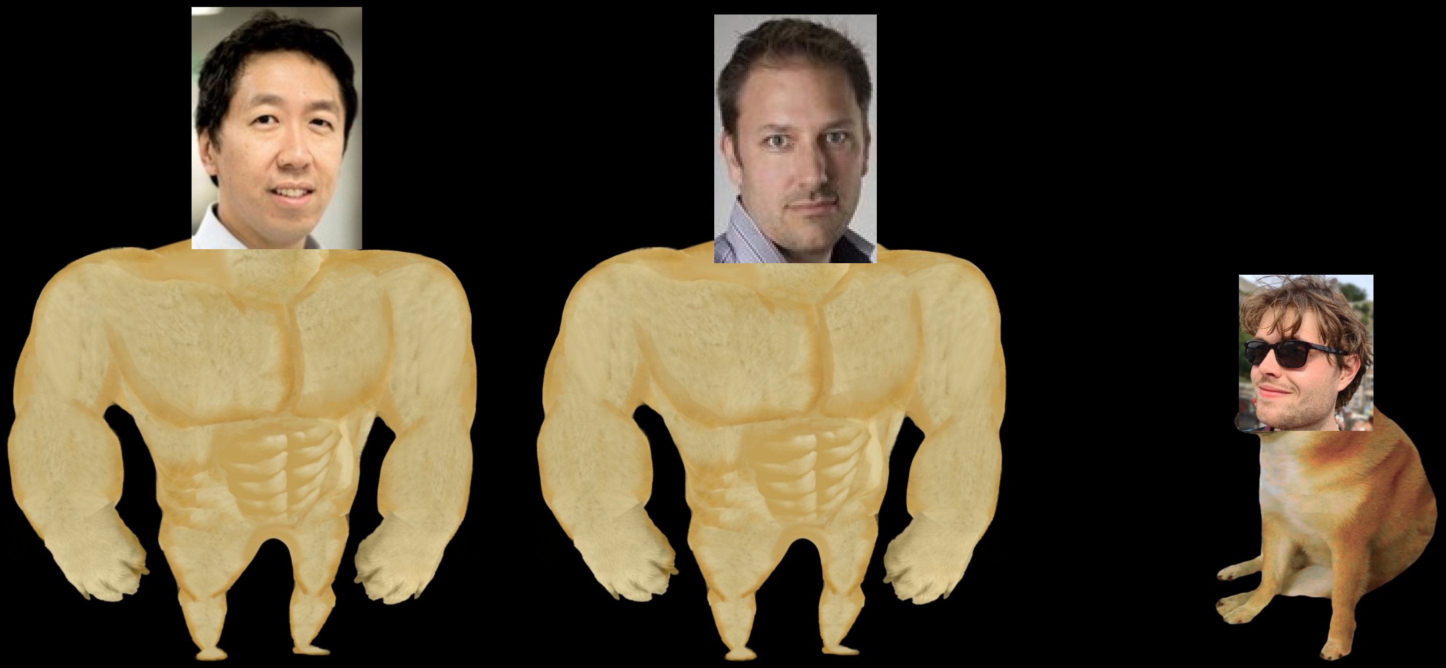
Why am I teaching this?

- ***I don’t know man, they told me to so I did it!***

Why am I teaching this?

- ~~I don’t know man, they told me to so I did it!~~
- Are you good at ML?
  - Like *good* good? No.
- Do you know more about ML than us?
  - *Maybe?* I sure hope so.
- This doesn’t help your credibility, you know
  - Sorry guys.

Real MVPs



Andrew Ng,
Coursera ML guru

Jeroen de Ridder,
resident ML
maestro UMCU

Dieter Stoker,
Some rando off
the streets

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.

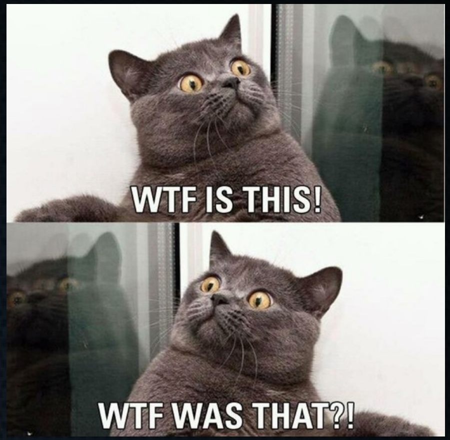
Setup per day

- 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

Lunch somewhere here
(12:15-13:00 is the idea)
Might shift times a bit.

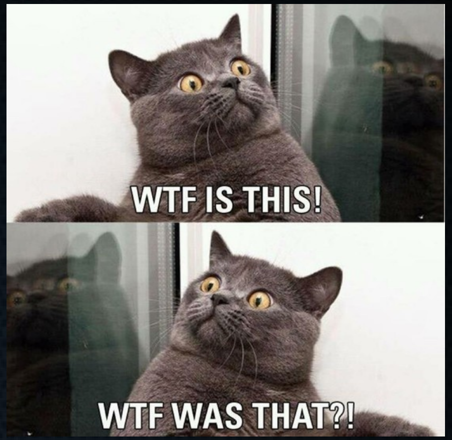
I need your help

- 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 it and give comments.
- In this way, I can hopefully take things on board quickly and perhaps change practicals or lectures during the course, rather than only after!



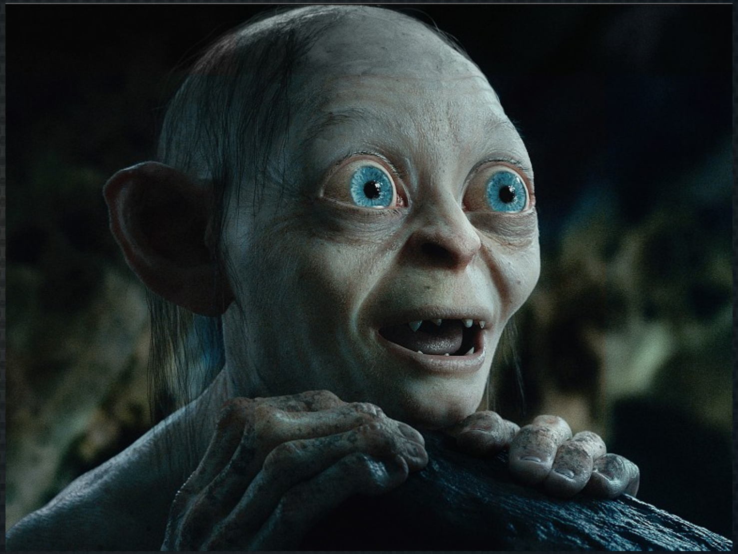
I need your help

- This is a new course. So probably, you’ll encounter difficulty spikes, things that don’t make sense, or other things that are lacklustre.
- This also means that we are going to discover together how much is reasonable to do:
  if there’s far too much material, say so, and
  we can scrap some!



I need your help 2

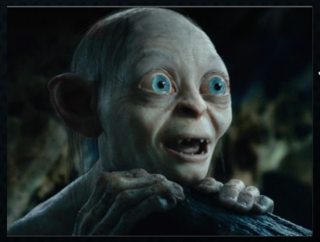
- You might wonder what's up with the coloured baubles I blessed you with.



I need your help 2

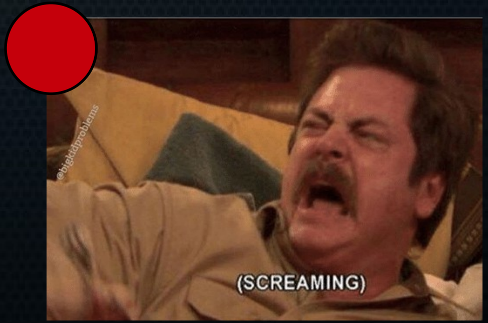
- You might wonder what’s up with the coloured baubles I blessed you with.
- They’re mood indicators for during the lecture:
  - Green: „I am positively brimming with enthusiasm to learn“ and/or „I can follow this material well enough“
  - Yellow/Orange: „This is somewhat difficult“ and/or „I feel my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

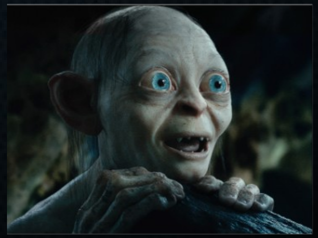





I need your help 2

- 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/address it, without you having to tell me to shut up. Win-win!





Questions

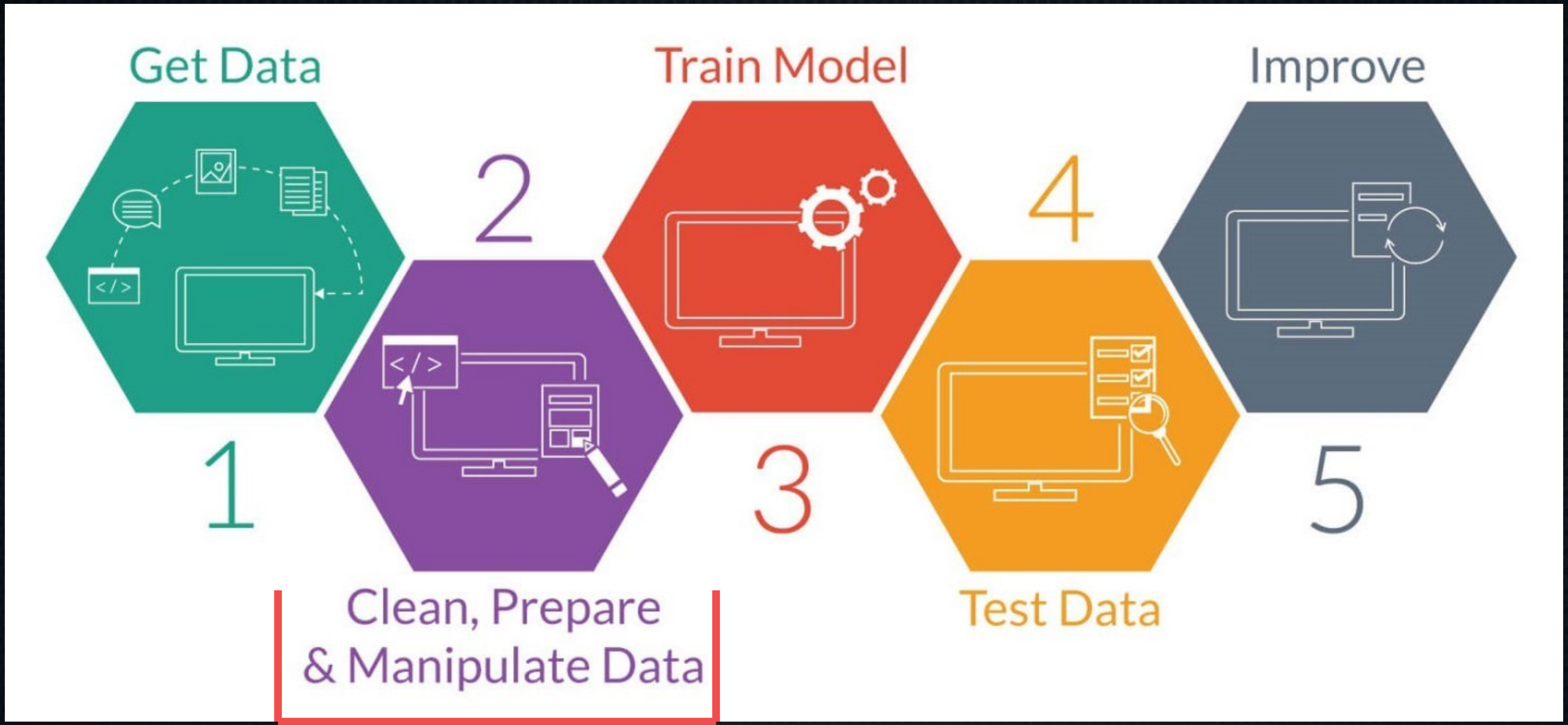
- Besides this, feel free to raise your hand and ask questions when something is unclear.

- If there’s no hands raised right now then we’ll dive right in!

This presentation

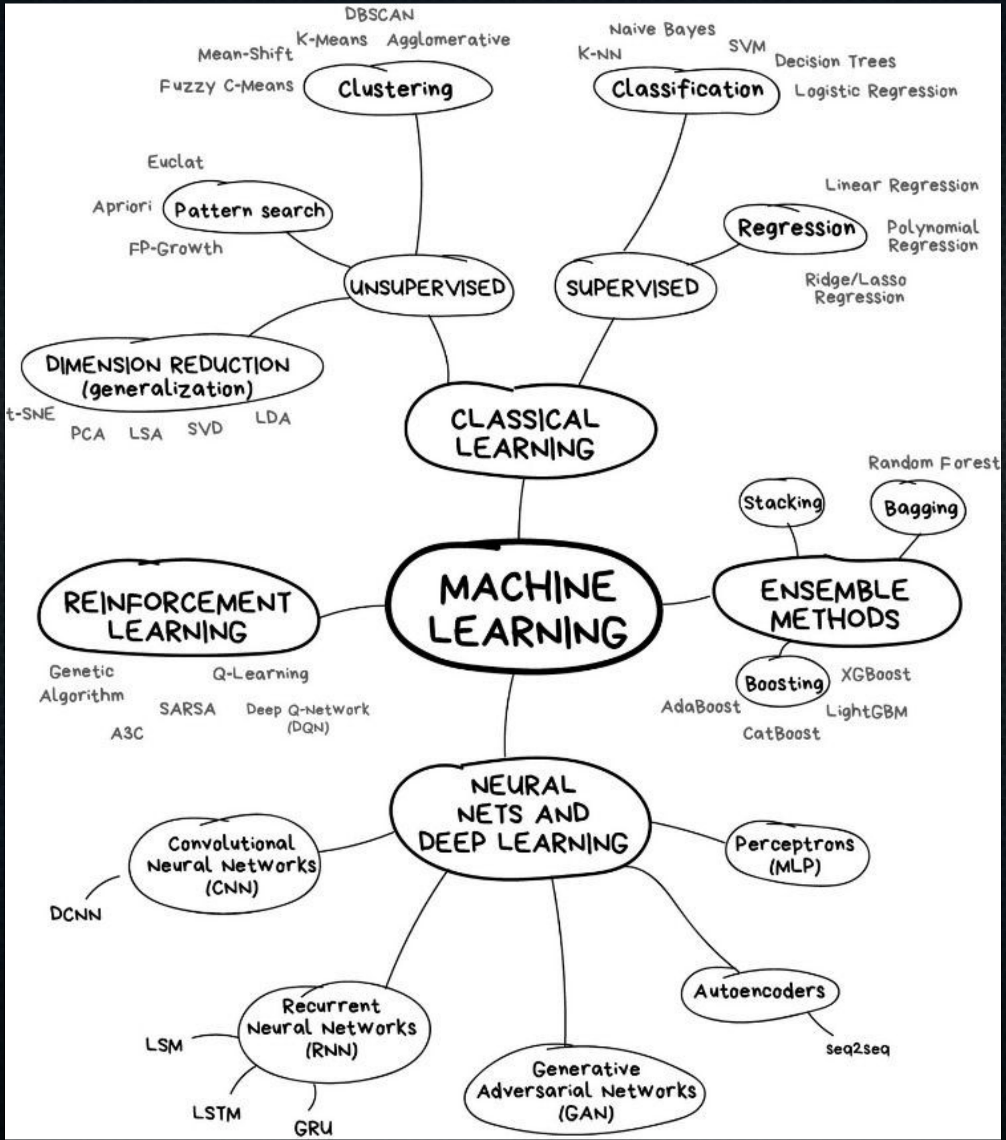
- Two branches of ML: supervised and unsupervised
- Terminology
- Linear regression & cost function
- Gradient descent & partial derivatives

The ugly truth about ML

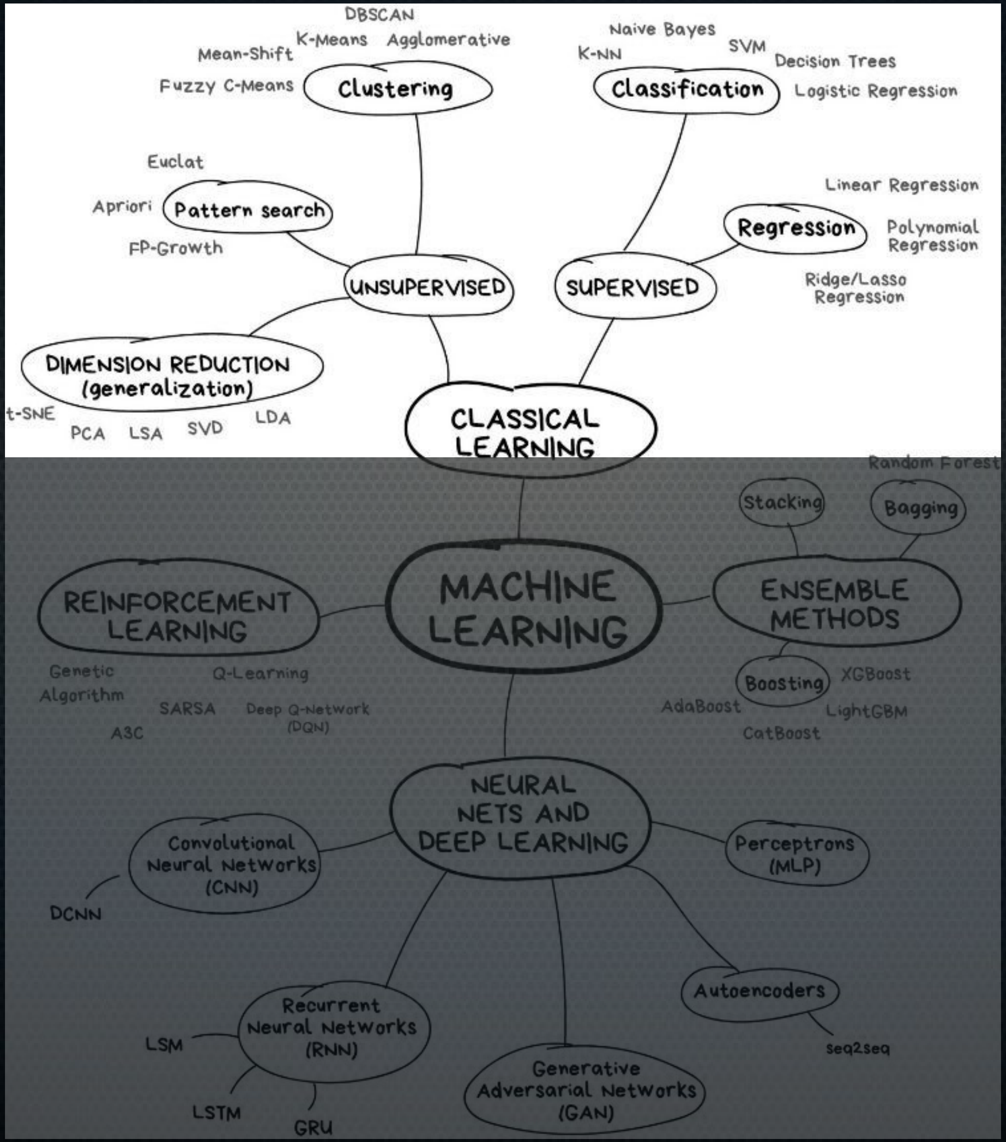


80% of your time

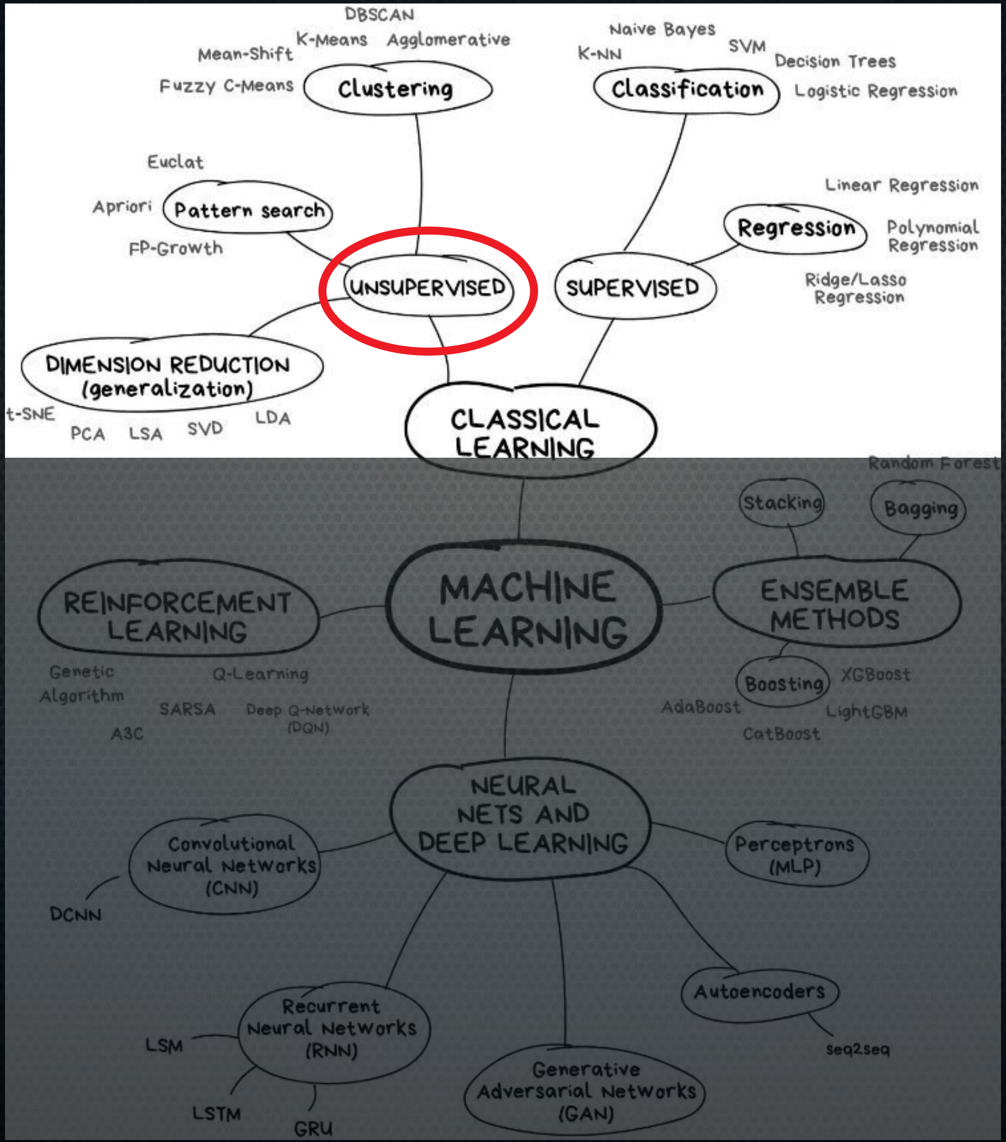
Map of Machine Learning



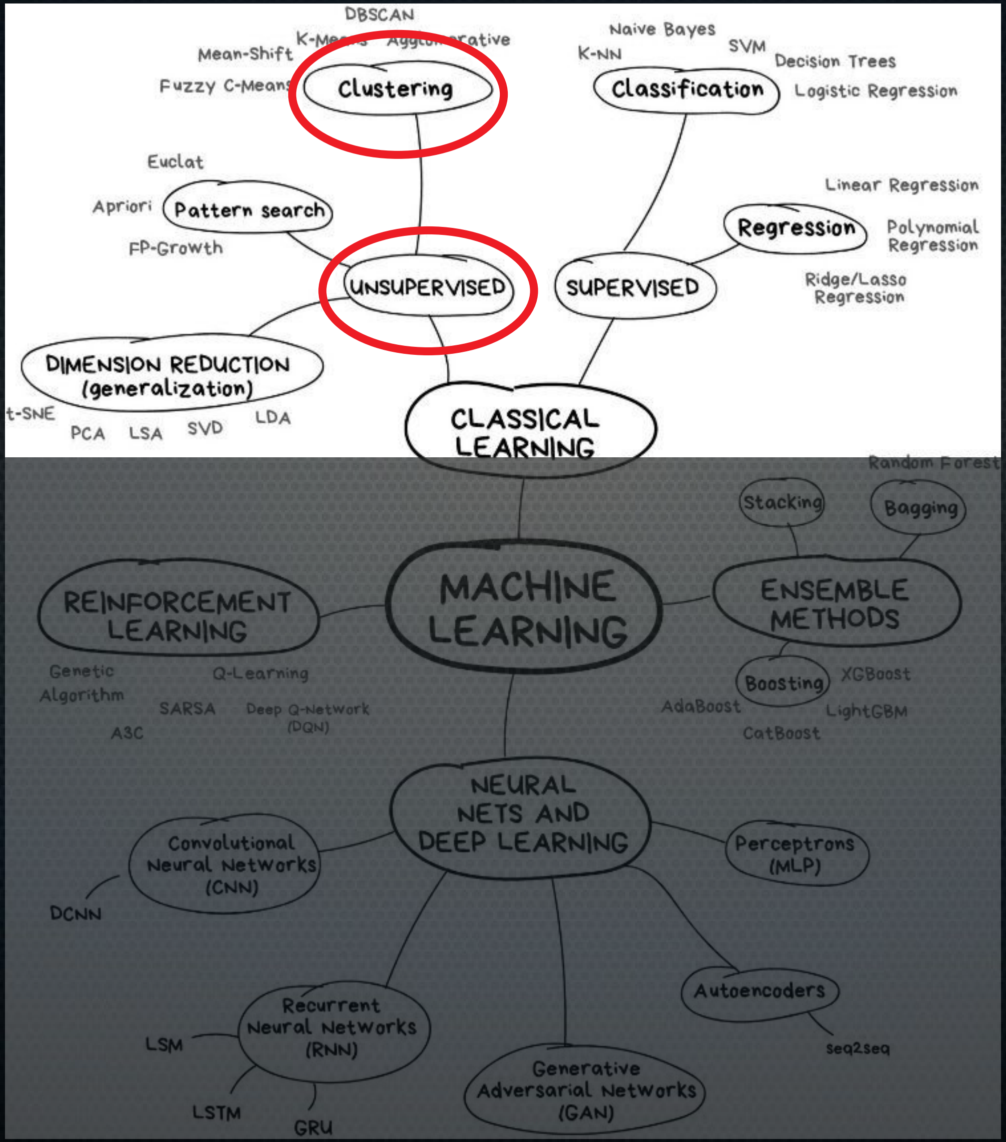
Map of Machine Learning



Map of Machine Learning

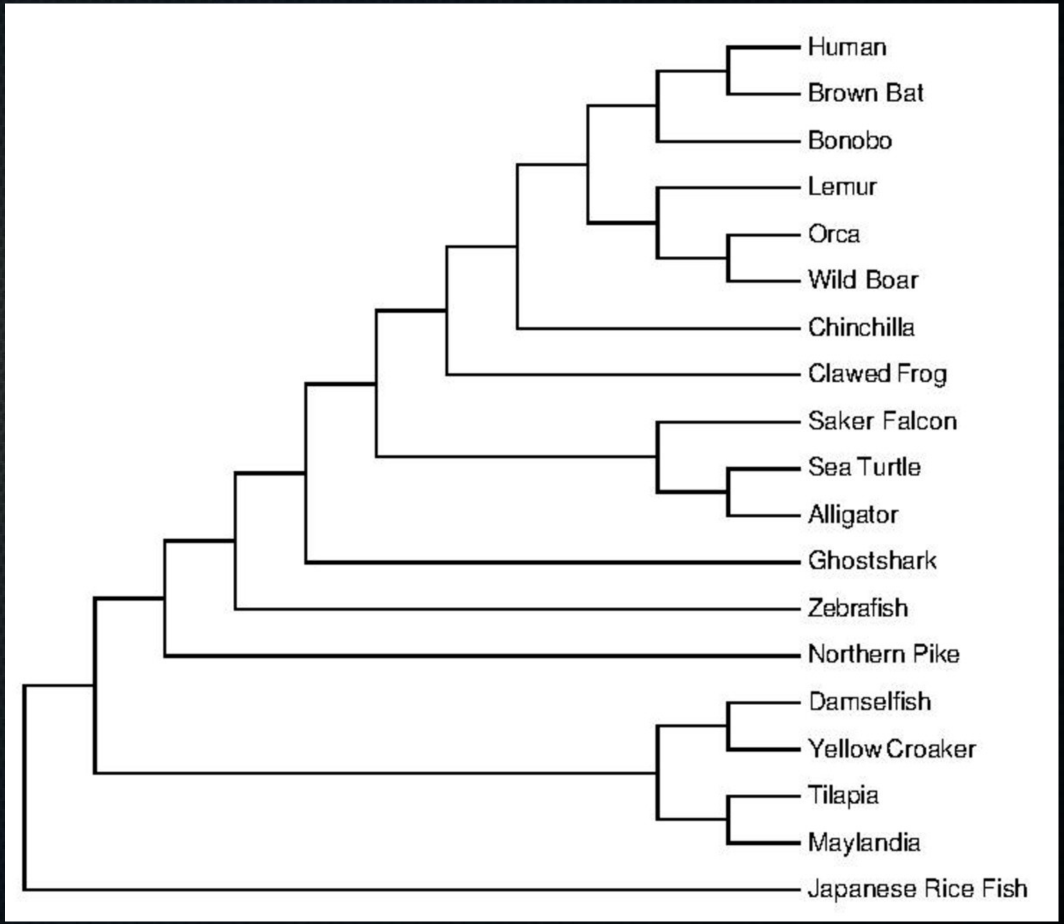


Map of Machine Learning



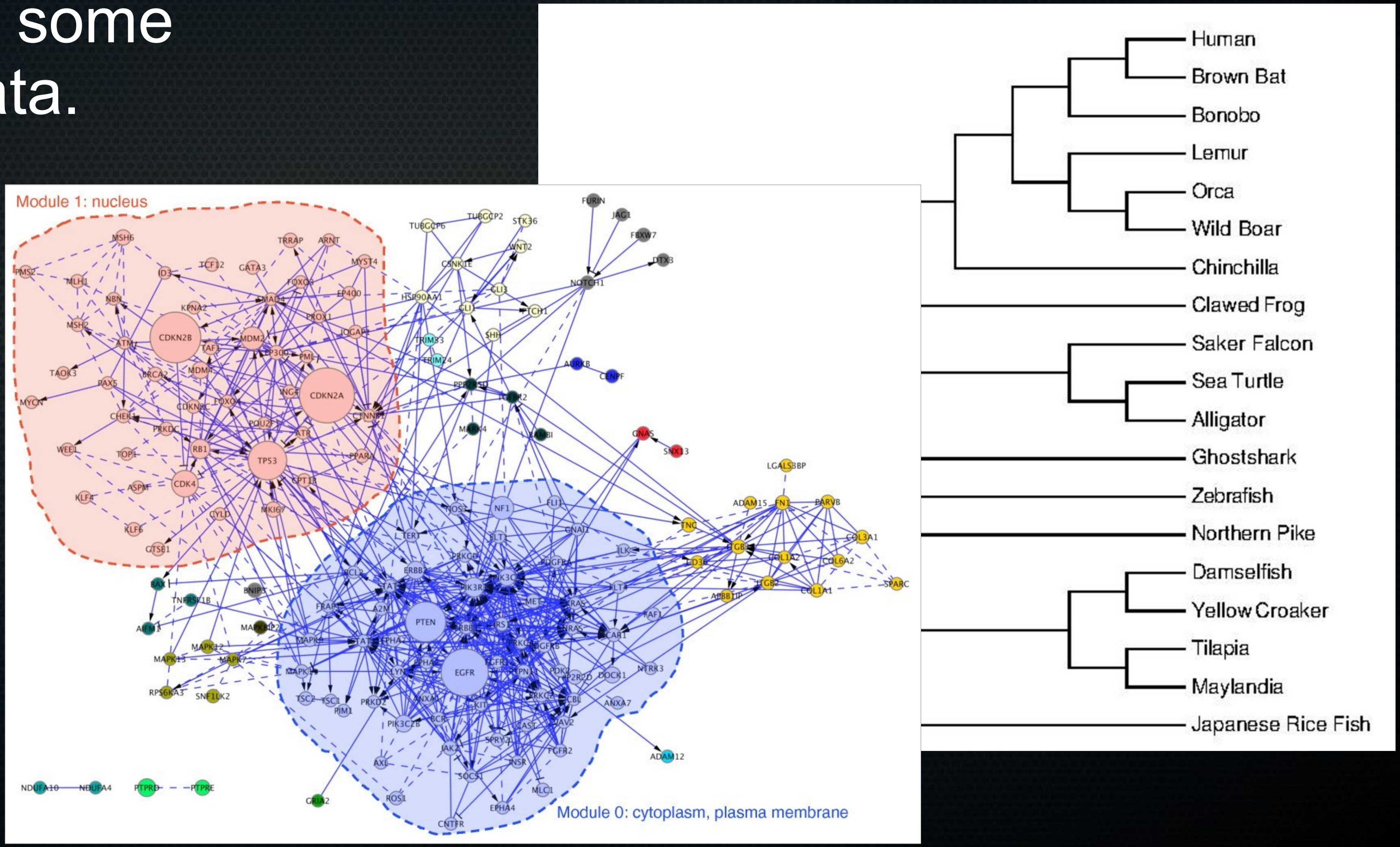
Unsupervised learning: clustering

- Automatically find some structure in the data.



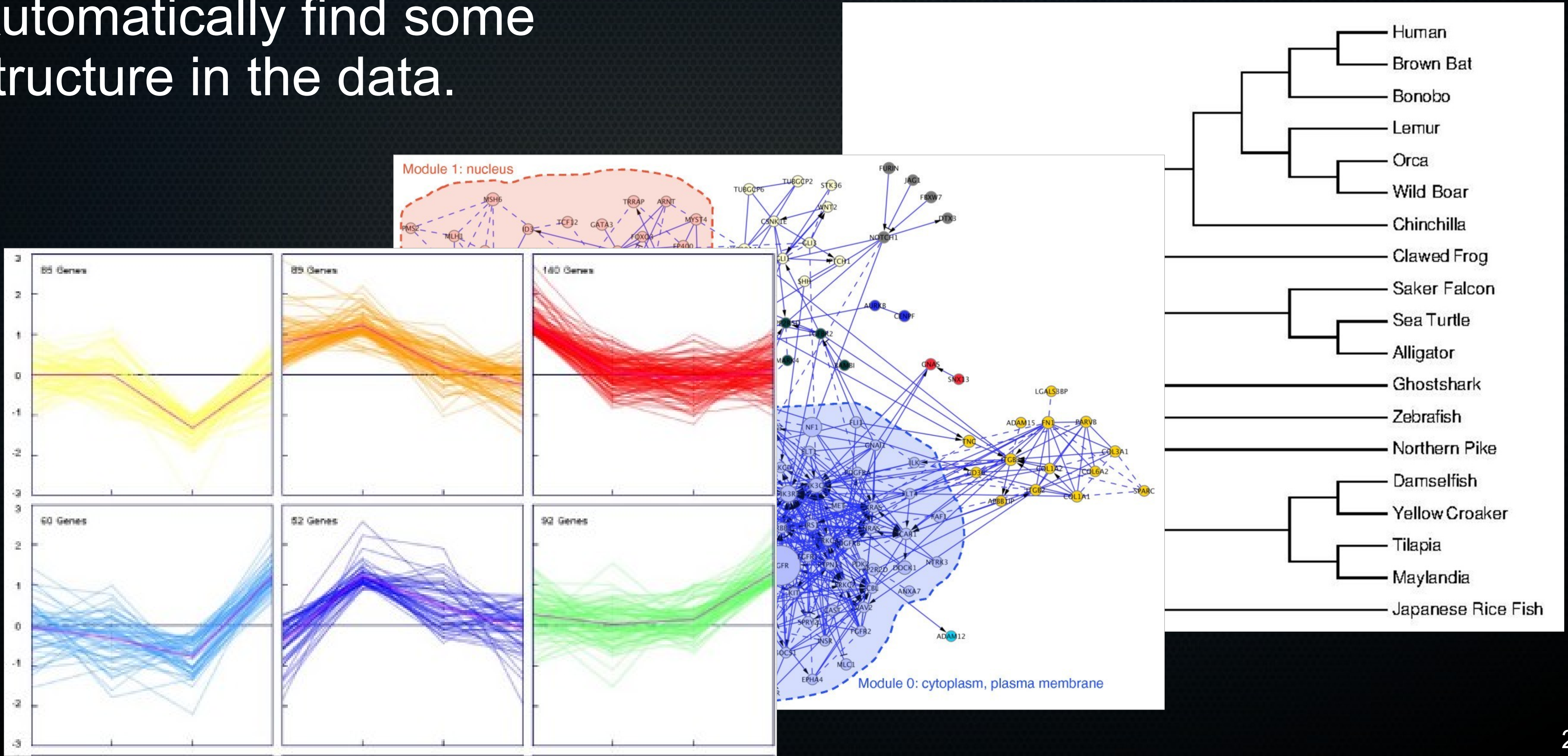
Unsupervised learning: clustering

- Automatically find some structure in the data.



Unsupervised learning: clustering

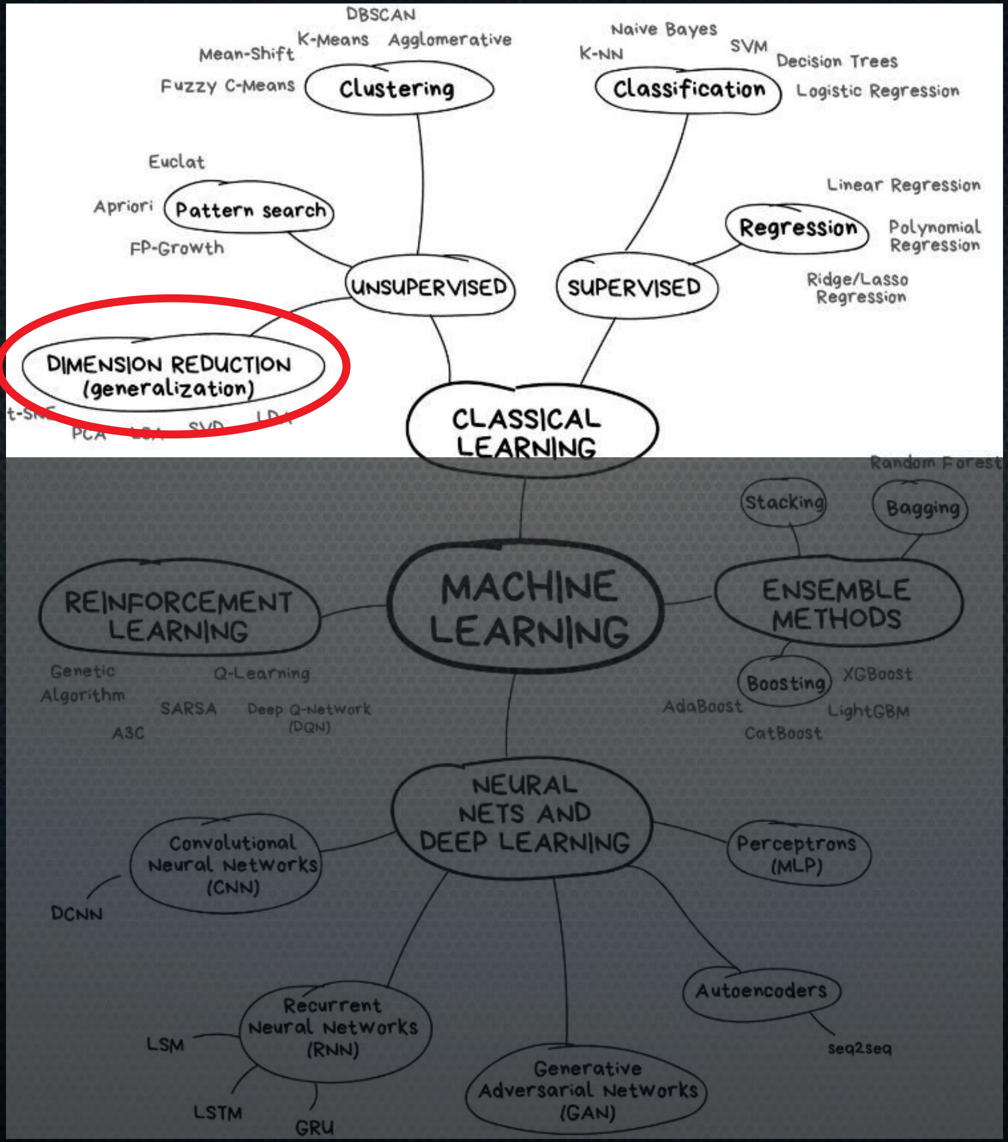
- Automatically find some structure in the data.



Unsupervised learning: clustering

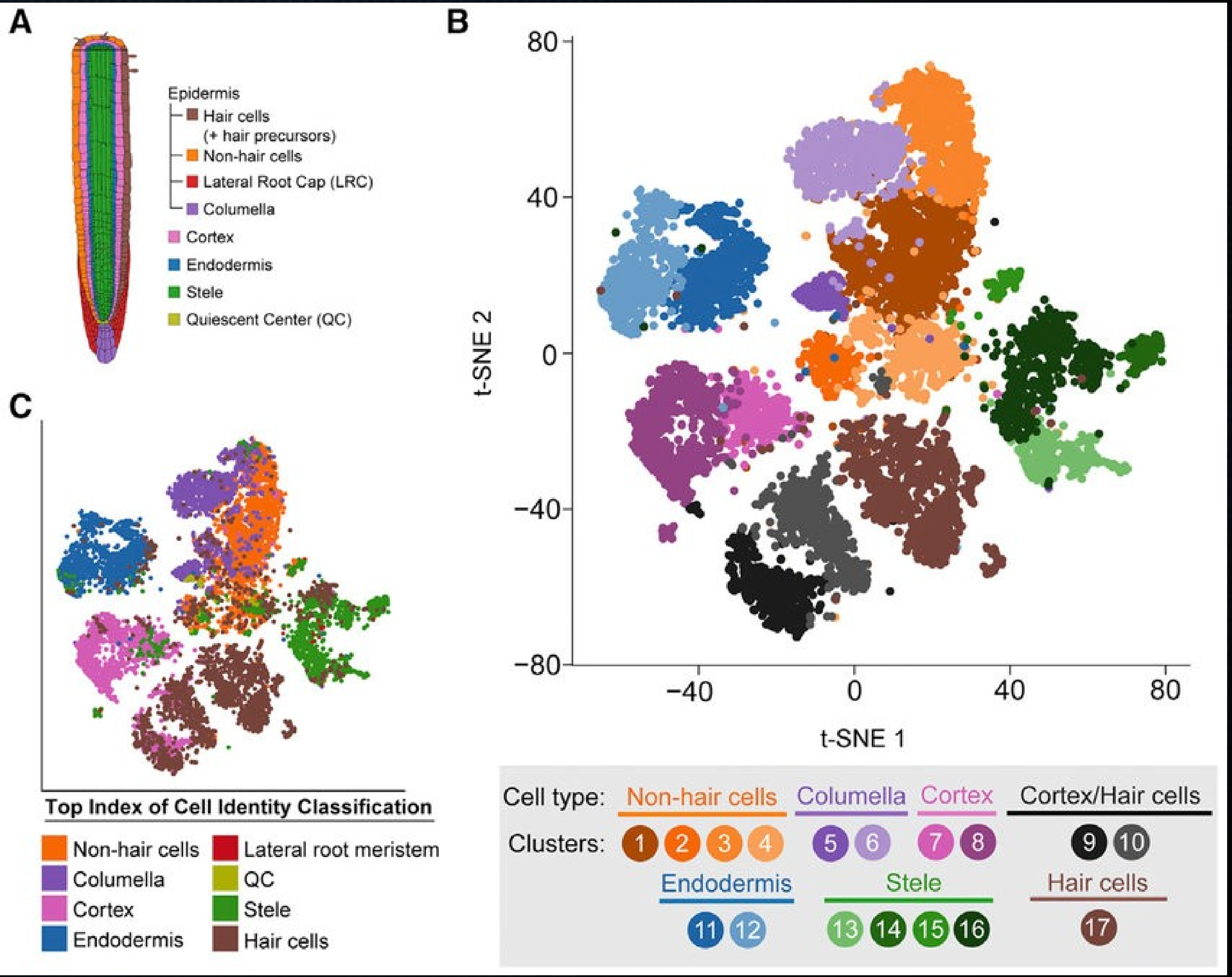
- No right or wrong:
  - Back-and-forth between different clustering algorithms, your knowledge, and the data.
  - You don‘t *know* correct clustering.

Map of machine learning



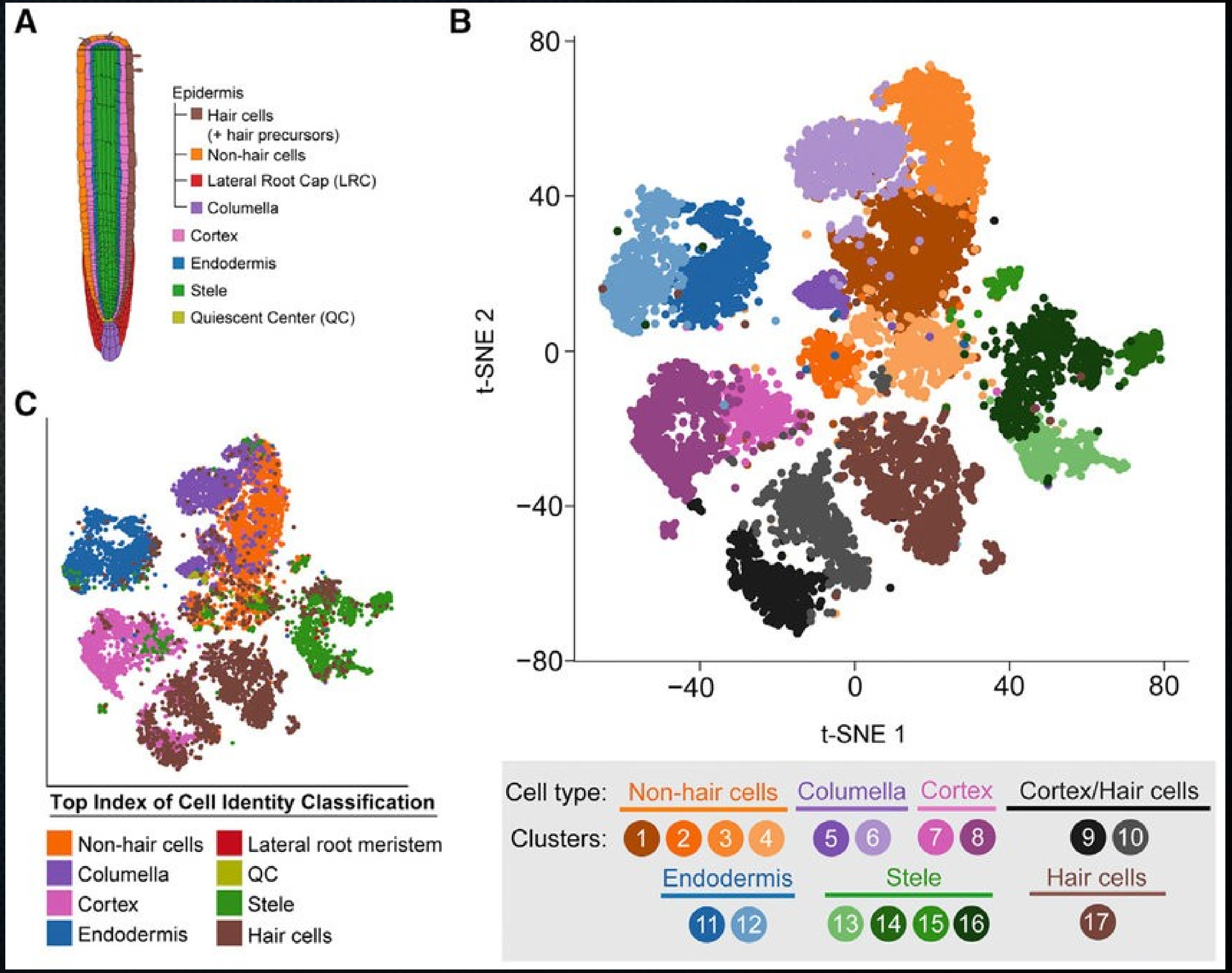
Unsupervised learning: dimensionality reduction

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



Unsupervised learning: dimensionality reduction

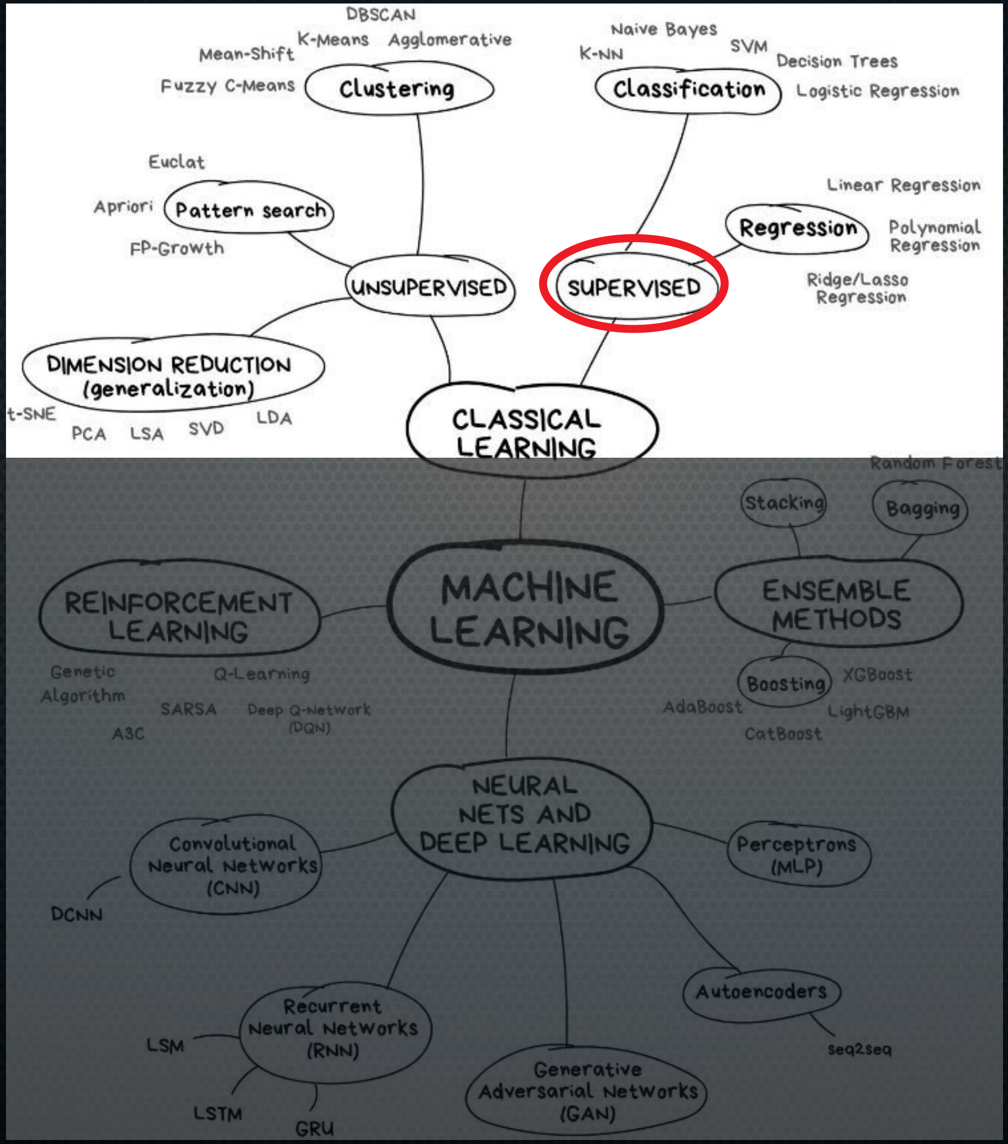
- Single-cell RNAseq of 12,198 Arabidopsis root cells.
- How do they differ?
- Visualise differences in all RNAs between all these cells in 2 dimensions.
- Used in conjunction with clustering (colours)



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)
  - Preventing overfitting and other ill effects of high dimensionality

Map of Machine Learning

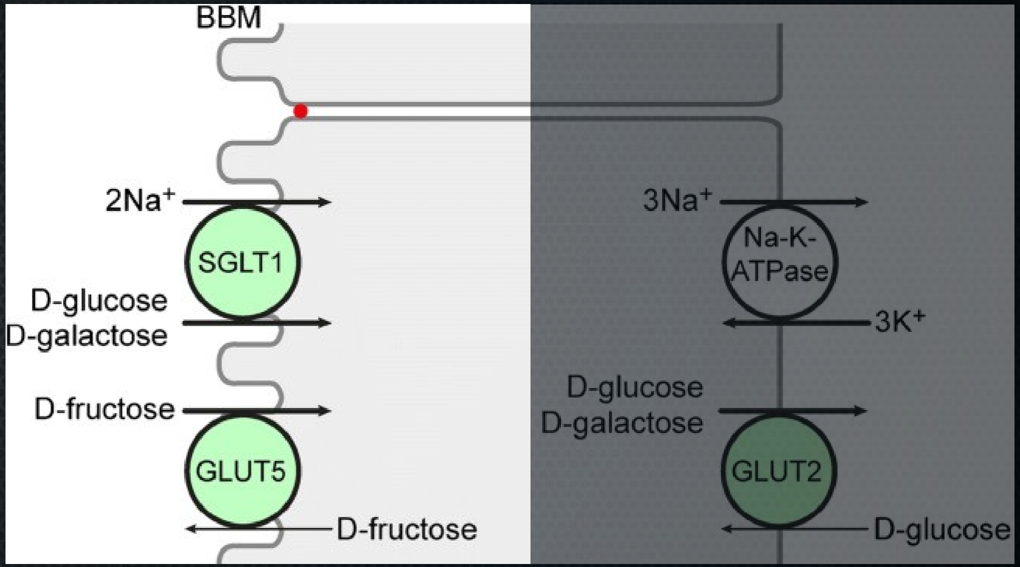


Supervised learning

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

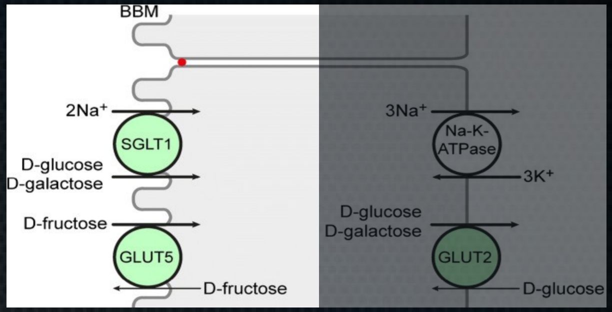
Supervised learning: regression

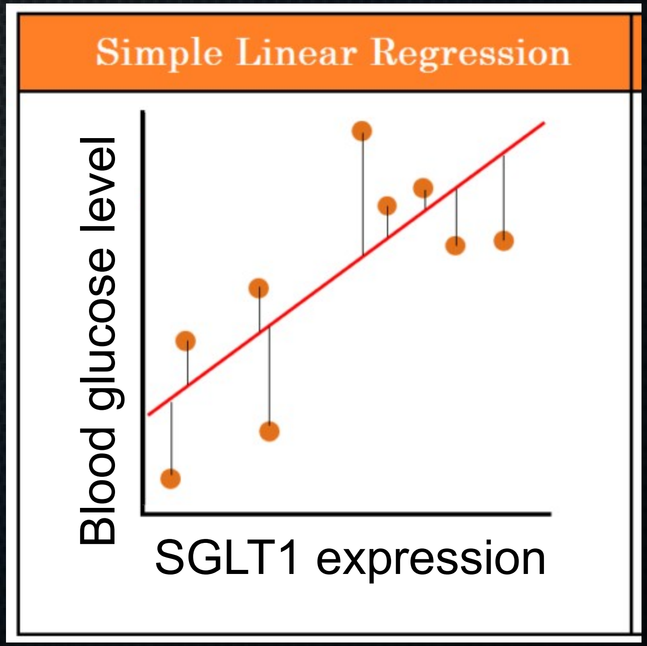
- Given known examples, automatically find a function to map new examples.
- Real-valued outputs.



Supervised learning: regression

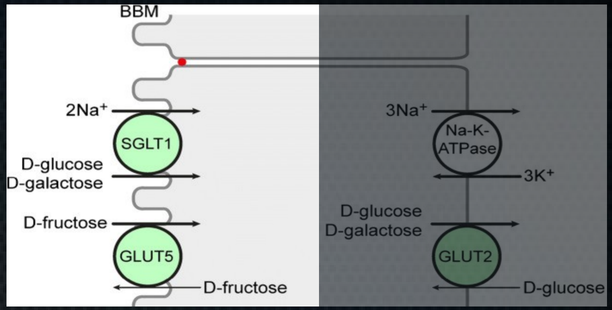
- Given known examples, automatically find a function to map new examples.
- Real-valued outputs.

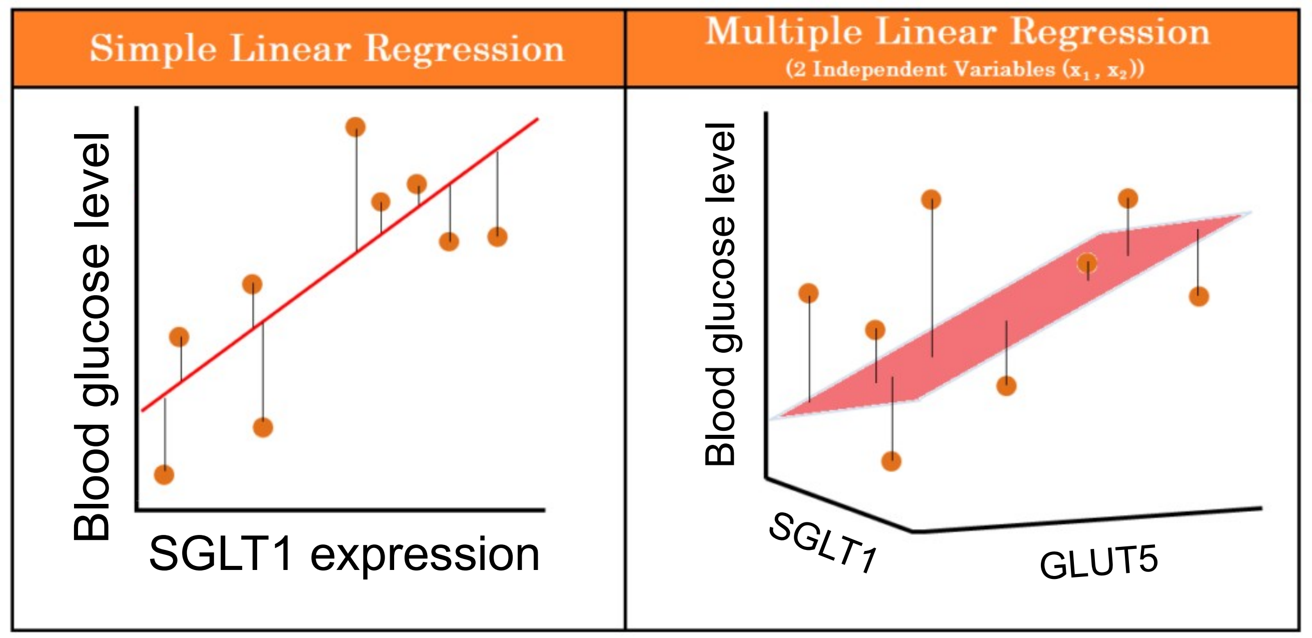




Supervised learning: regression

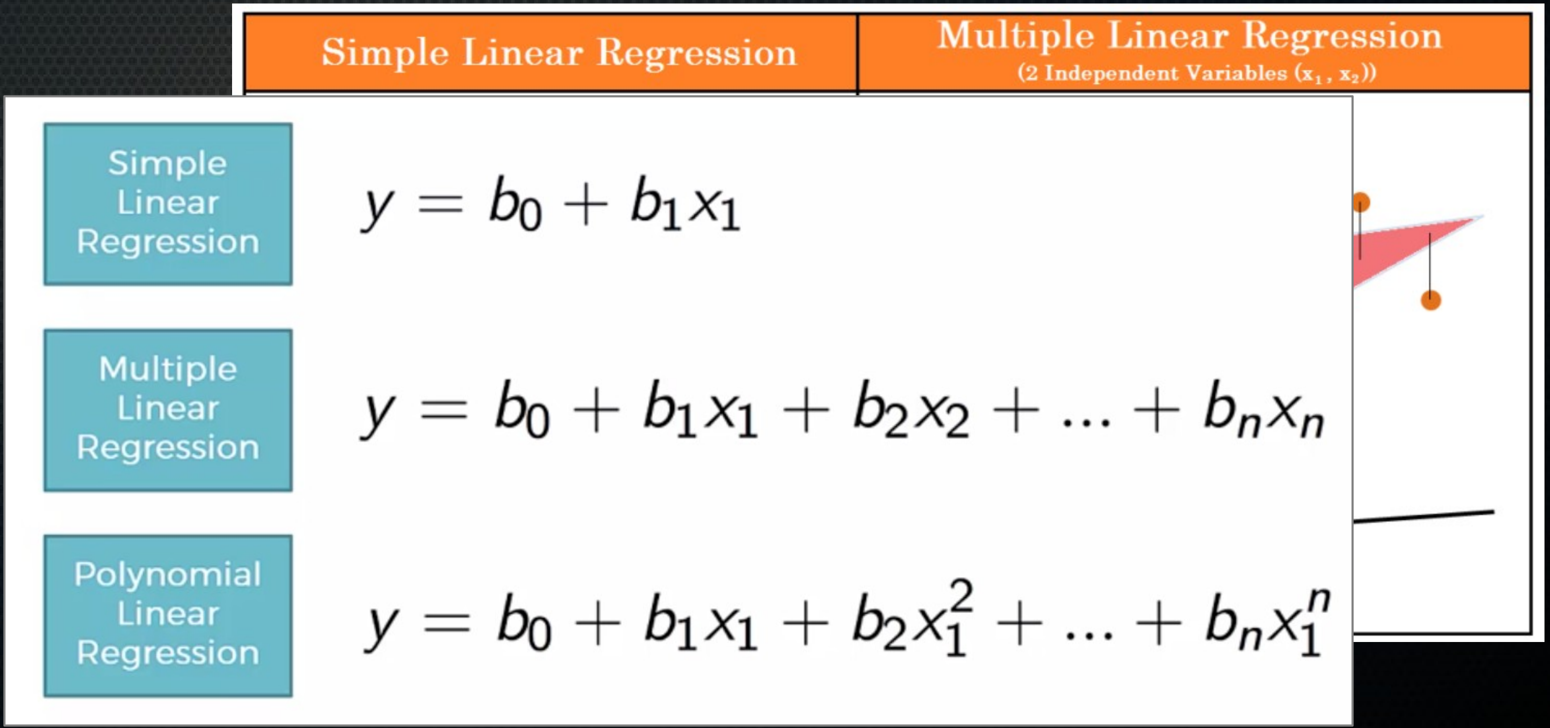
- Given known examples, automatically find a function to map new examples.
- Real-valued outputs.





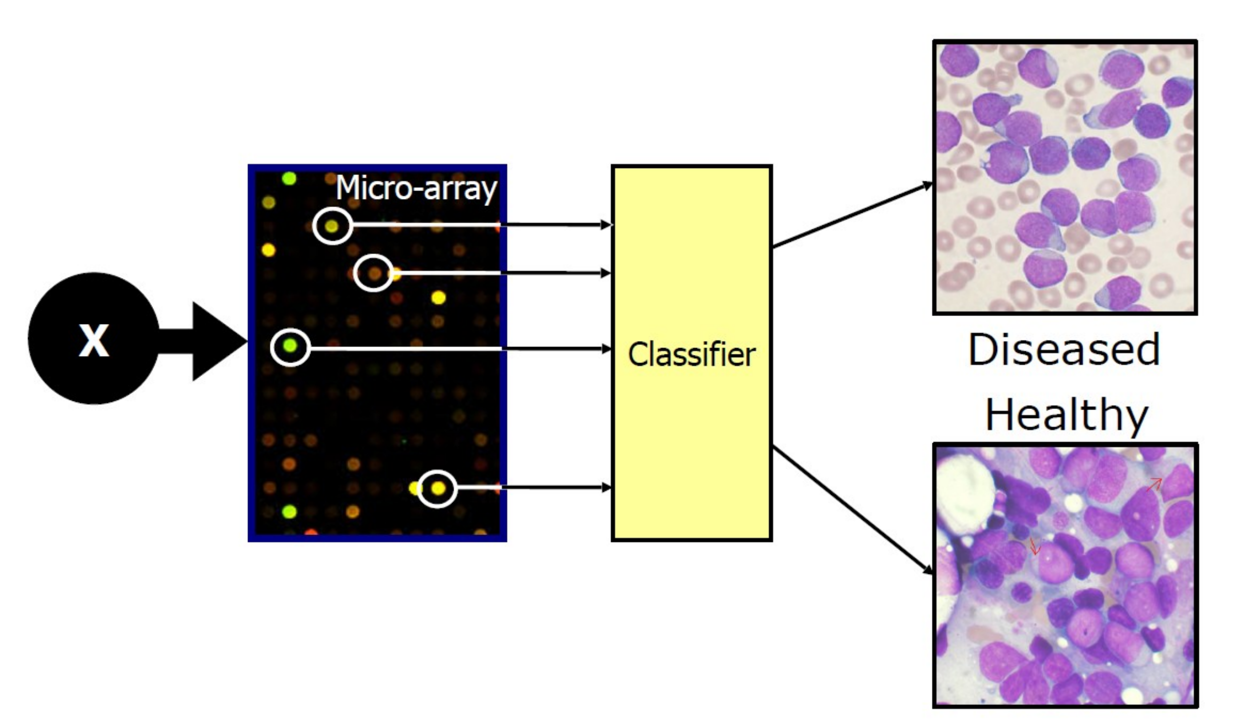
Supervised learning: regression

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



Supervised learning: classification

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



Source: Jeroen de Ridder

Supervised learning: classification

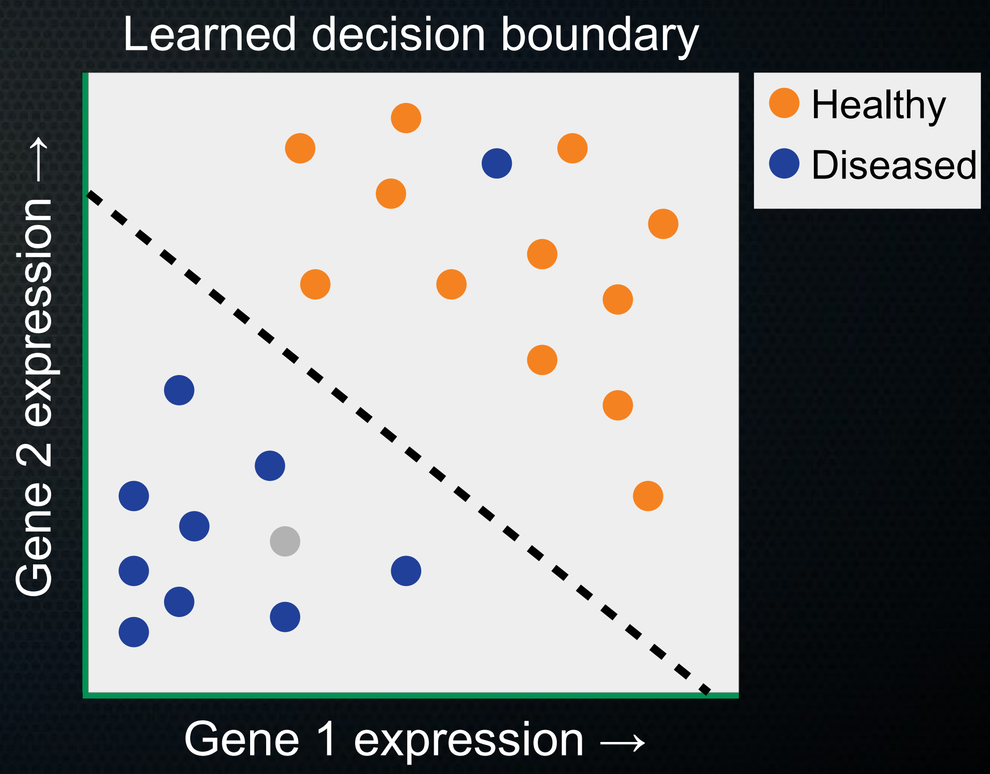
- Given known examples, automatically find a function to map new examples.
- Discrete outputs.

Supervised learning: classification

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

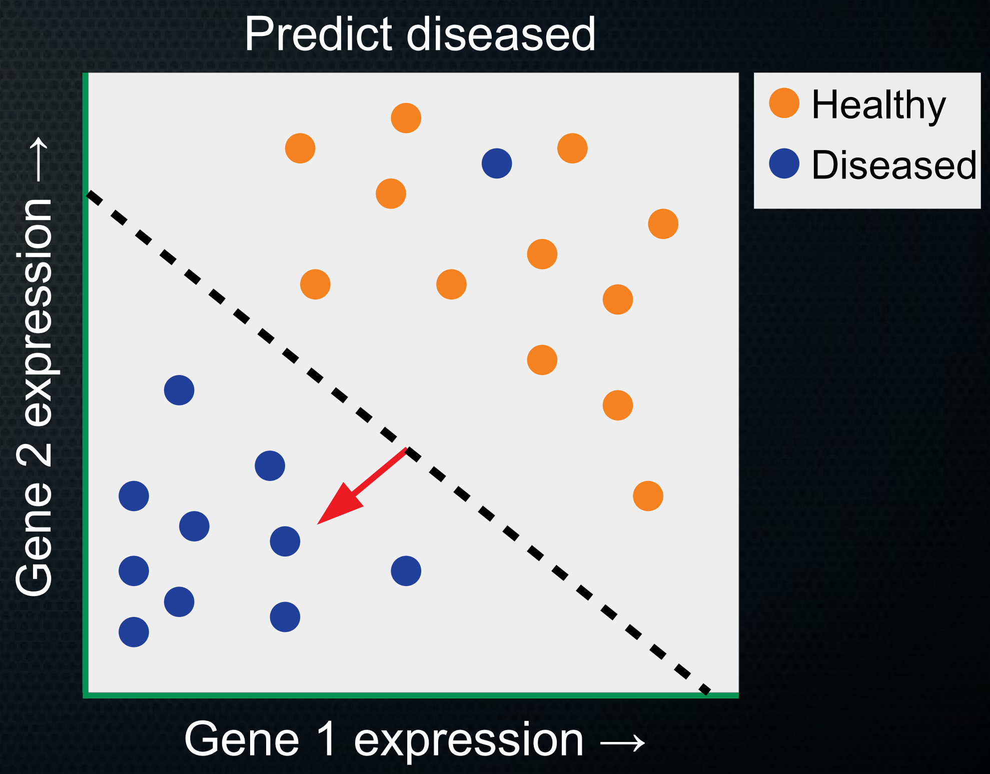
Supervised learning: classification

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

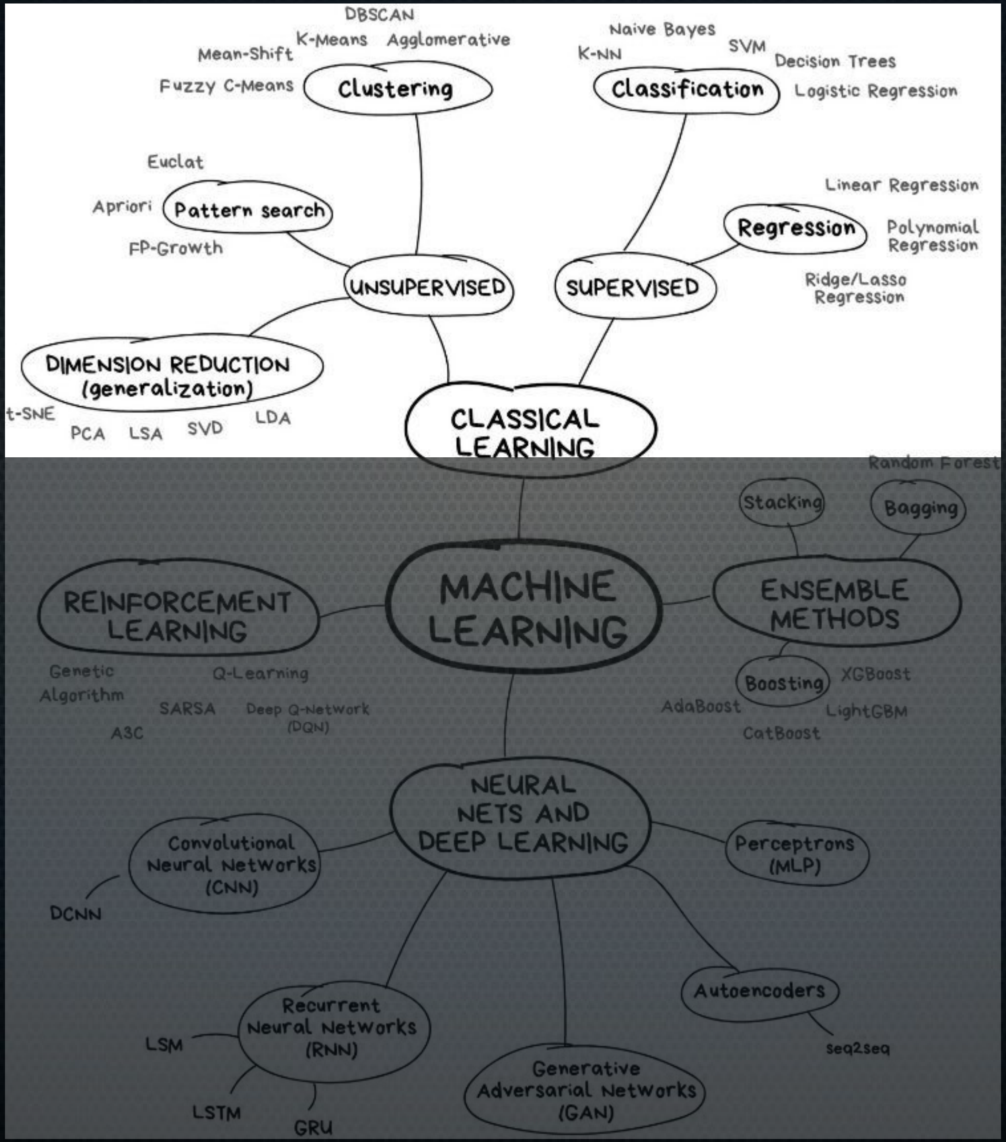


Supervised learning: classification

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



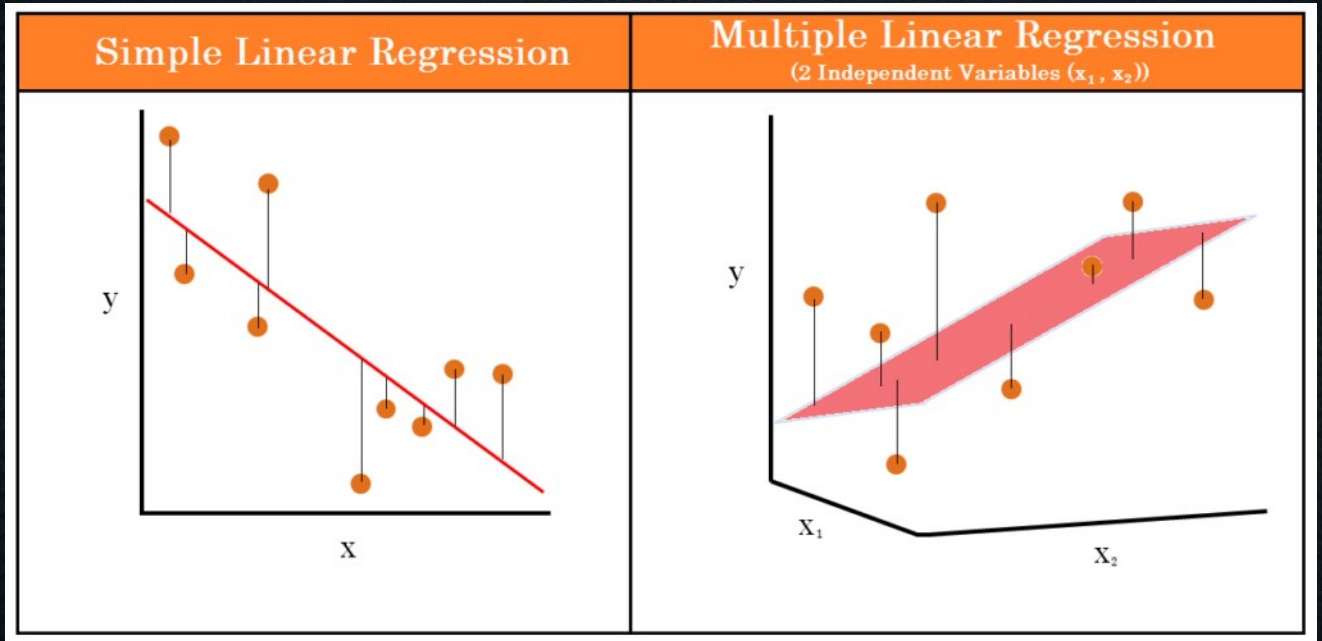
Map of Machine Learning



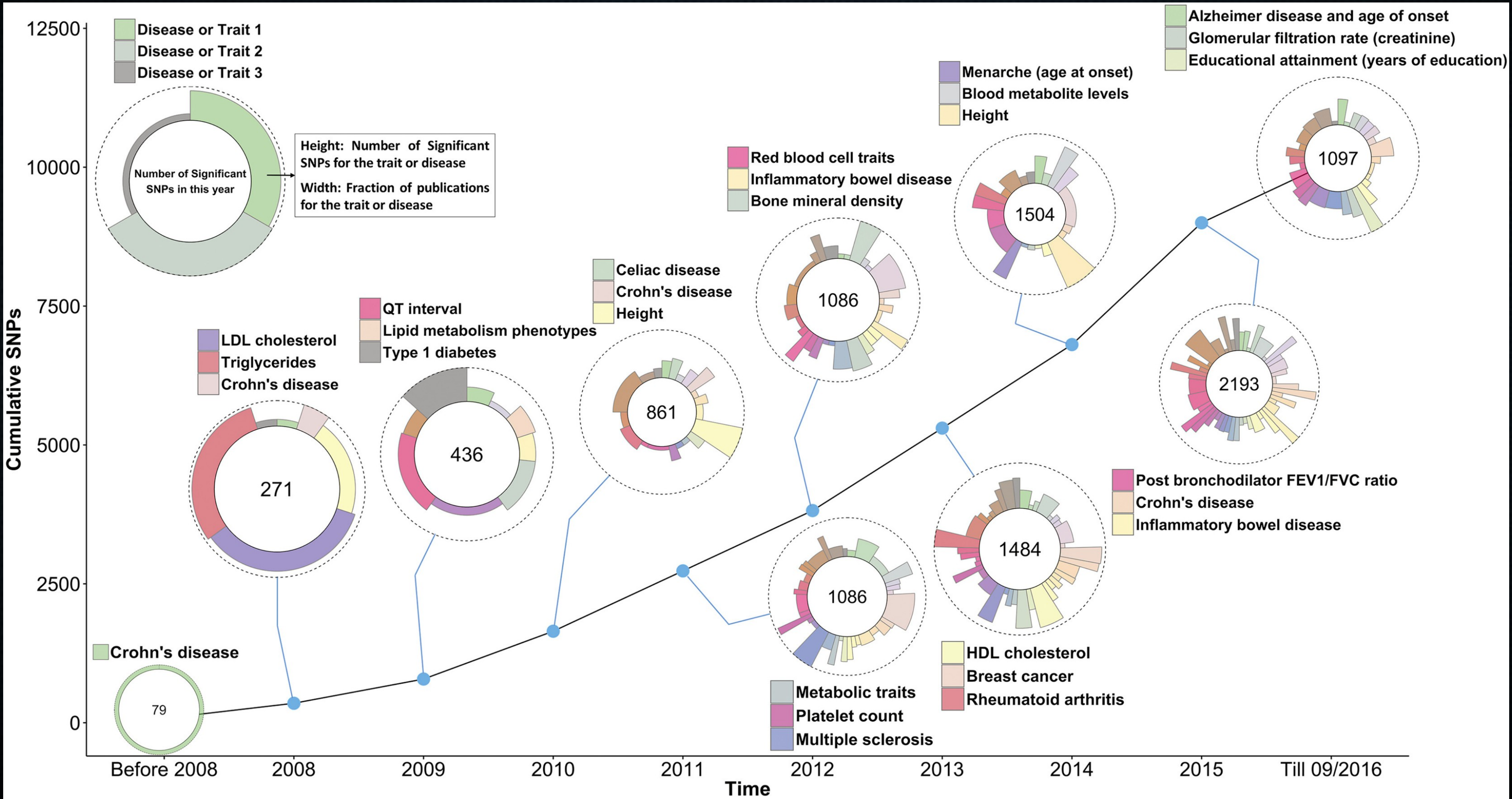
Summary

- Unsupervised:
  - Find some structure in your data (clusters, projection into lower-dimensional 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.

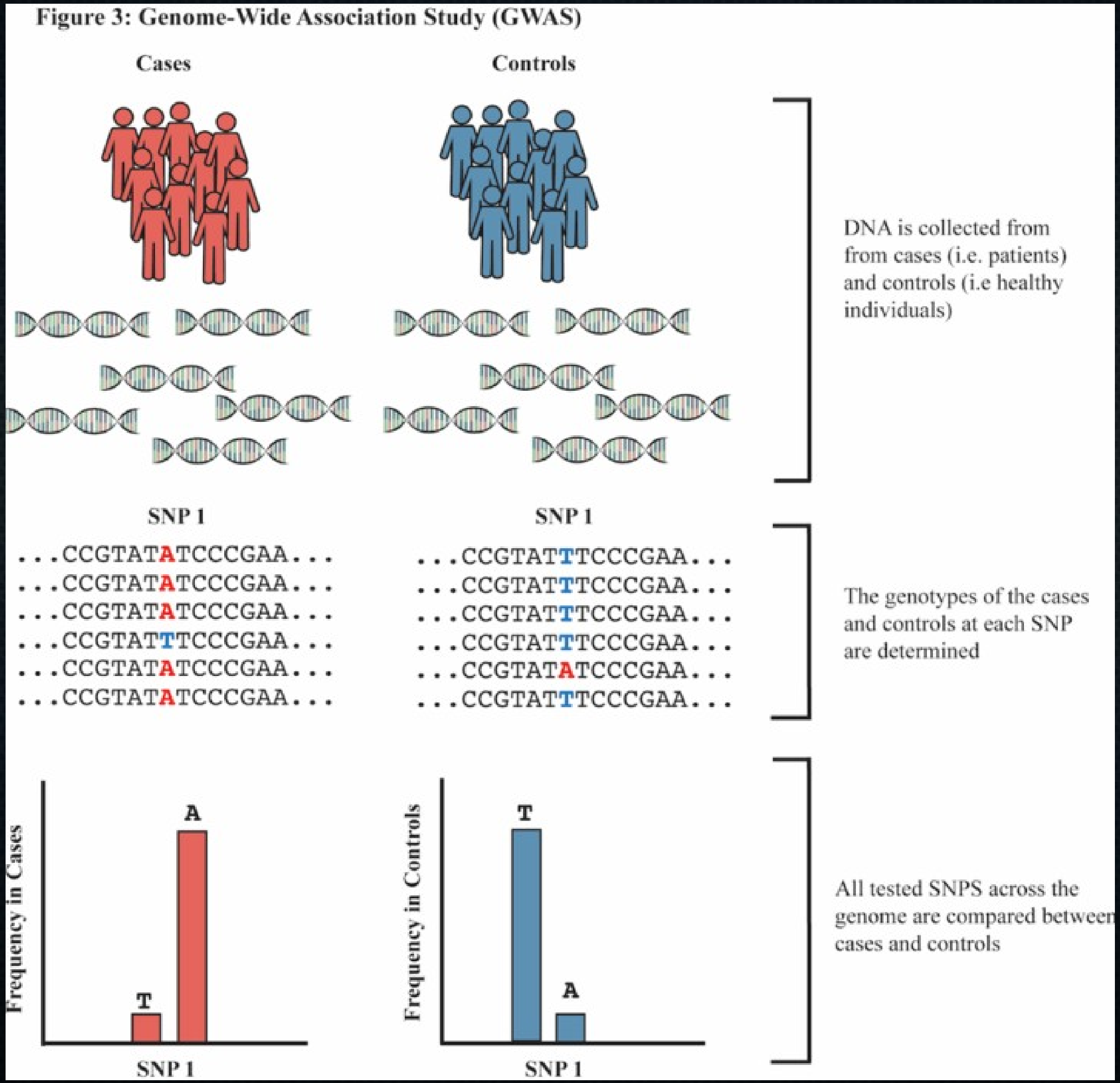
Linear regression



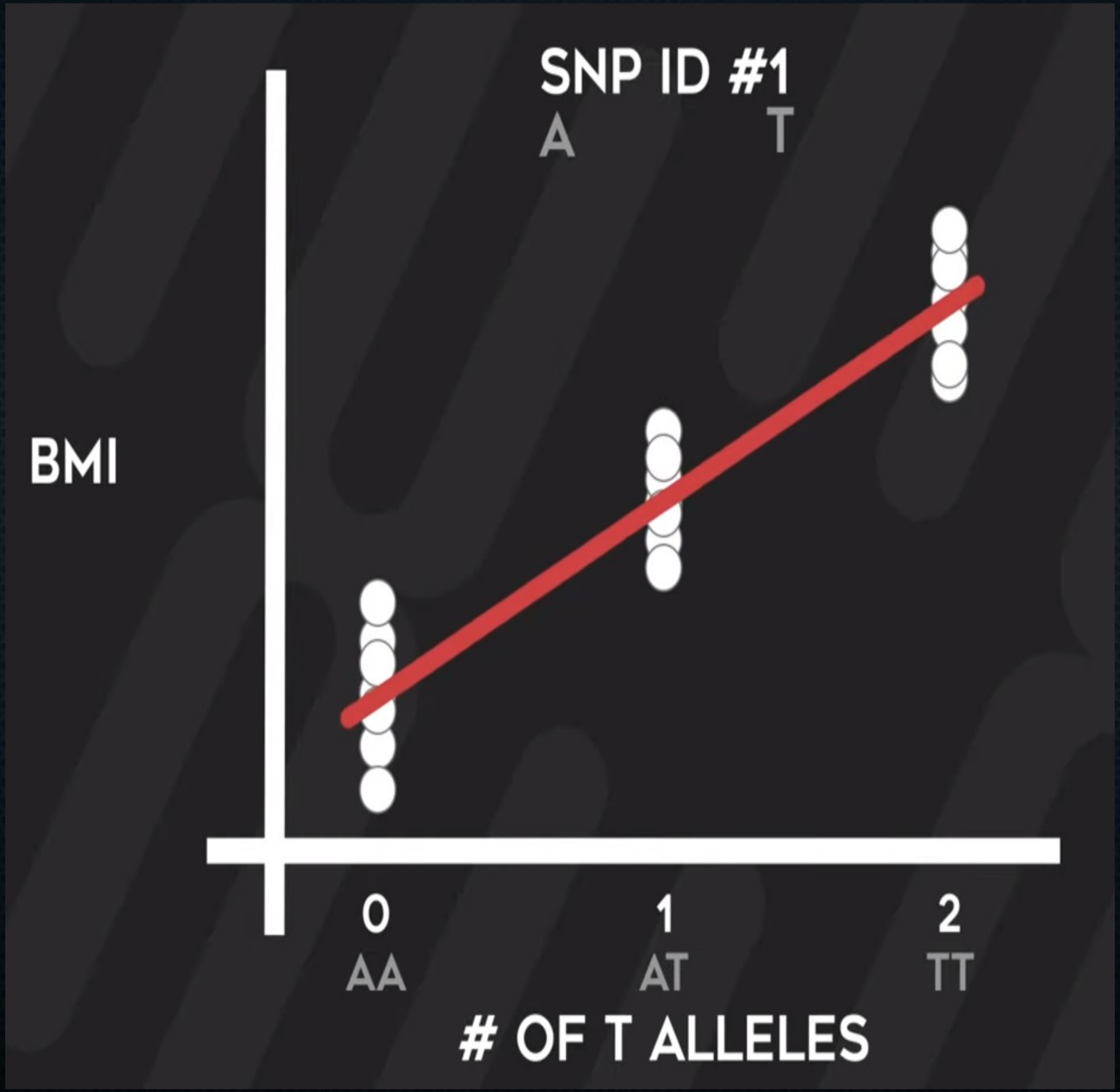
Linear regression: GWAS



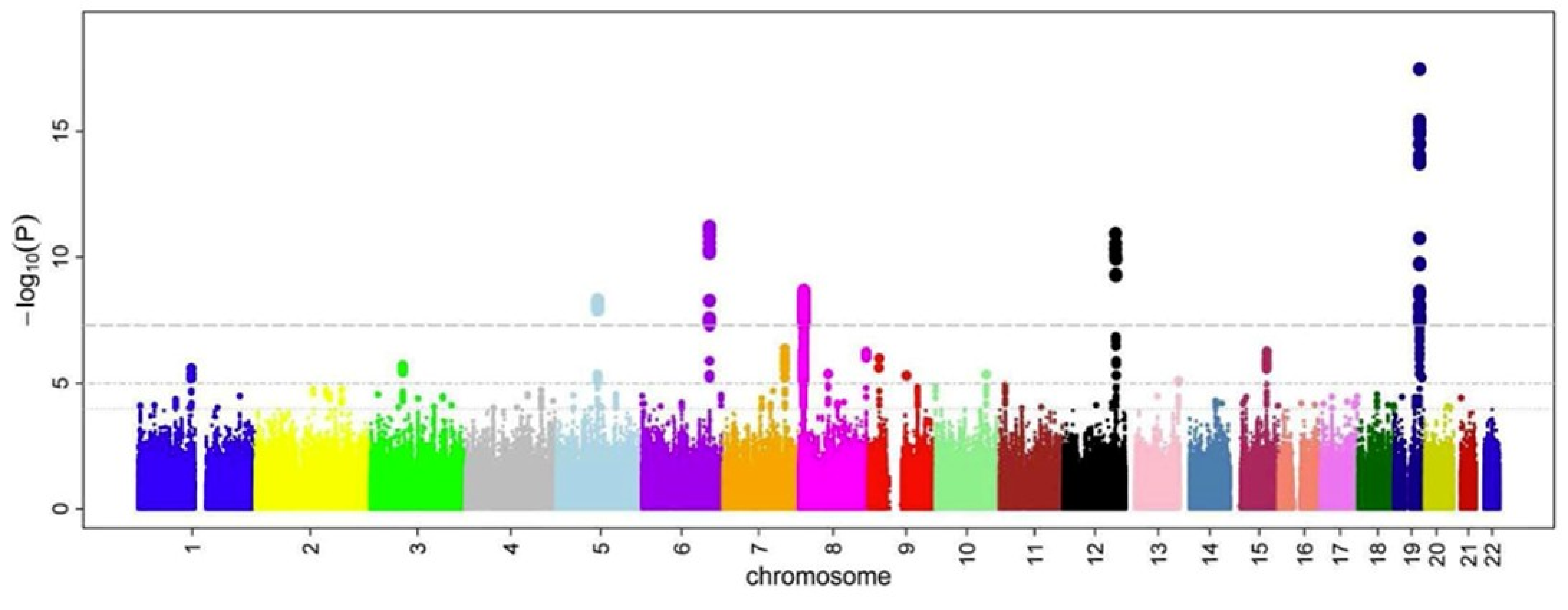
Linear regression: GWAS



Linear regression: GWAS



Linear regression: GWAS



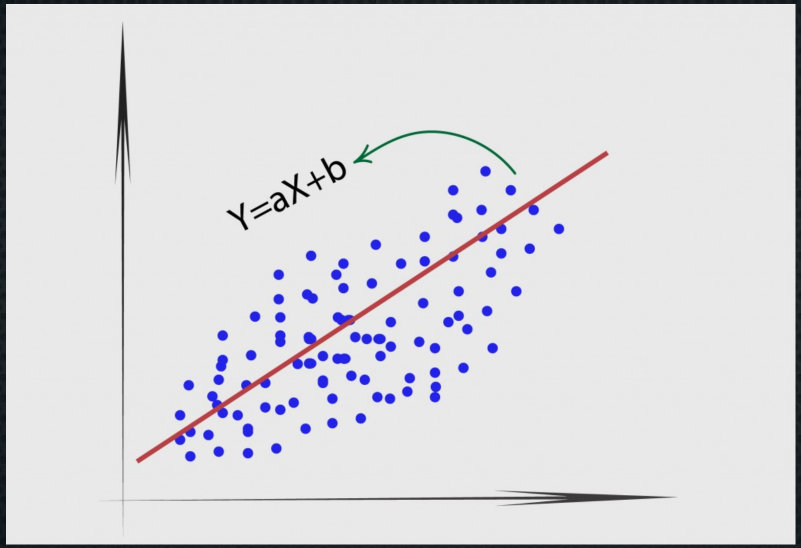
Linear regression: GWAS

- 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

$y = ax + b$

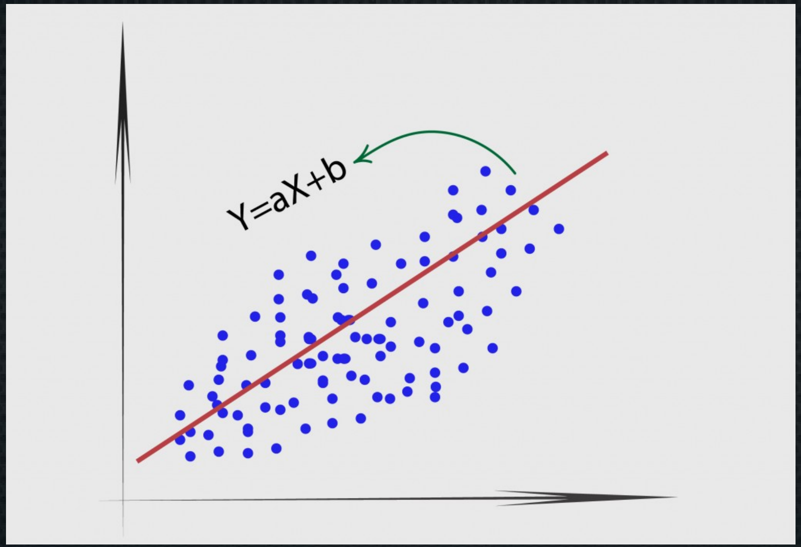
$$y = ax + b$$



Univariate linear regression

$y = ax + b$

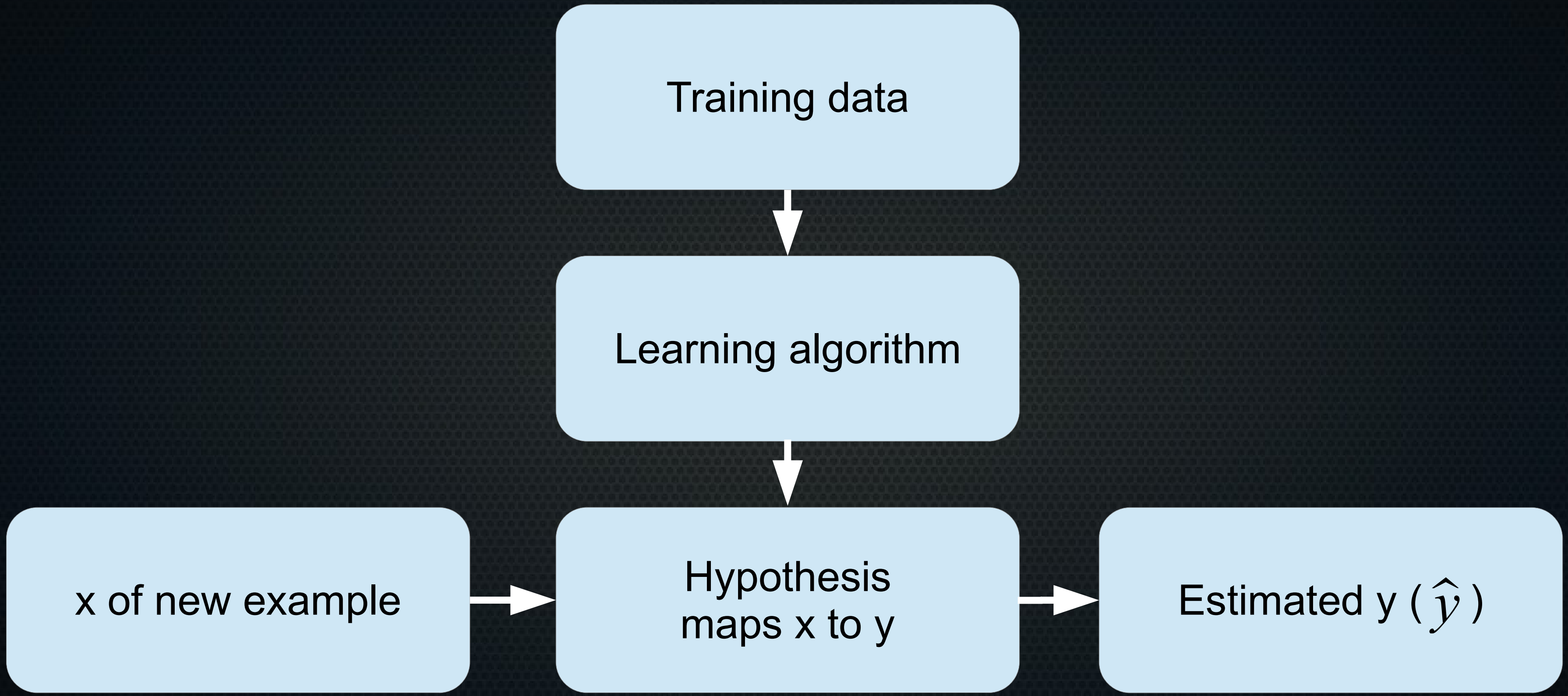
$$y = ax + b$$



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

Process

$y = ax + b$

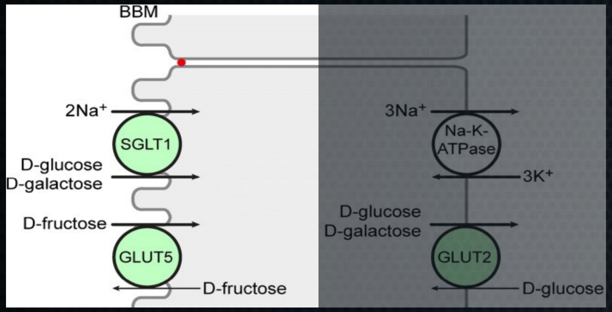


Source: Andrew Ng, Coursera

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

Terminology

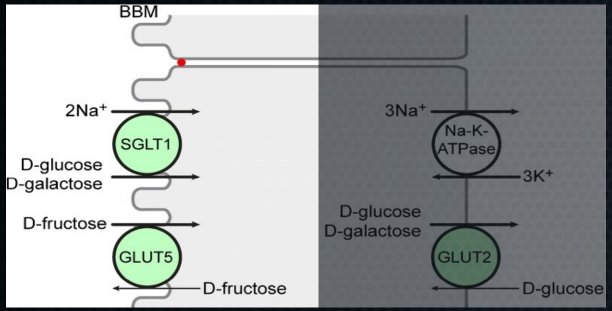
Training data



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

Terminology

Training data



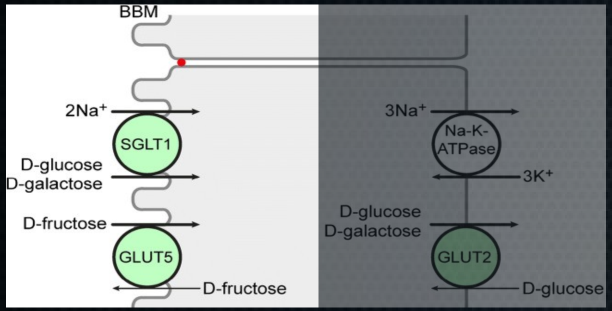
m = # of training examples

m

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

Terminology

Training data



m = # of training examples
n = # of features/variables

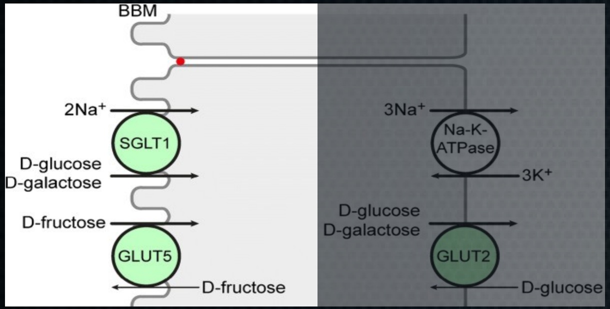
m

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

n

Terminology

Training data



m = # of training examples
n = # of features/variables

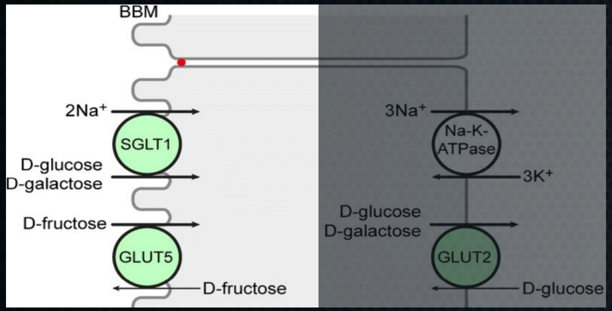
Sample #	x1	x2	x3	Blood glucose level (mg/dL)
1	3	2	11	80
2	8	3	2	130
3	12	4	666	170
4	2	6	5	89

m

n

Terminology

Training data



m = # of training examples
n = # of features/variables
y = output variable/target variable or label (classification)

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

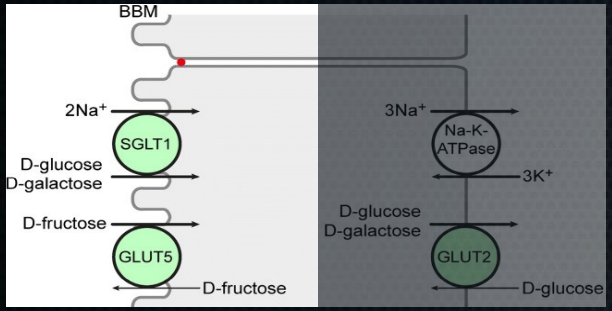
m

n

y

Terminology

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

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

m

$(x^{(3)}, y^{(3)})$

n

y

Cost function and gradient descent

$y = ax + b$

- 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?

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

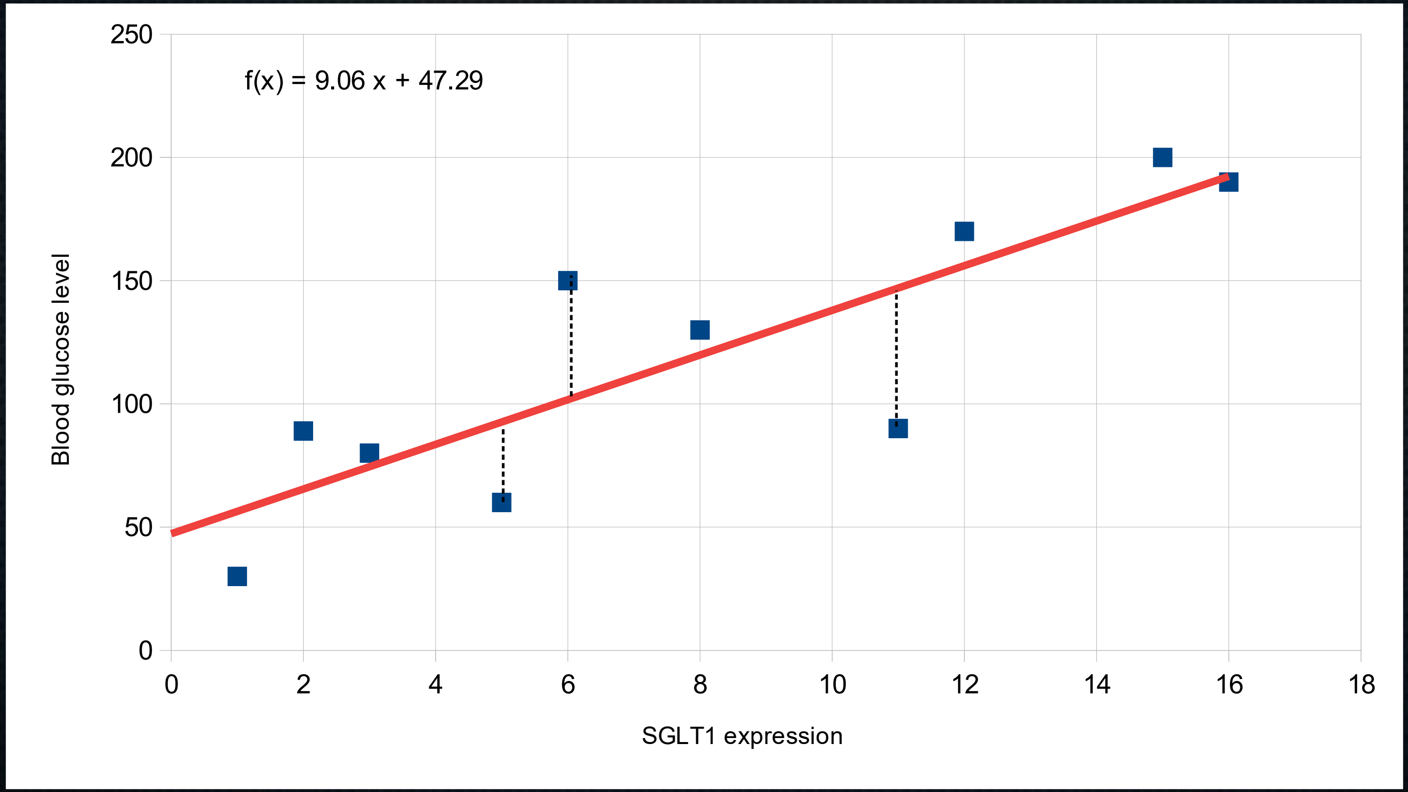
Cost function and gradient descent

- How to learn theta‘s from data?
- Two parts
  - ***<u>How wrong are we for given parameters?</u>***
  - How do we update our parameters, given how wrong we are?

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

Cost function

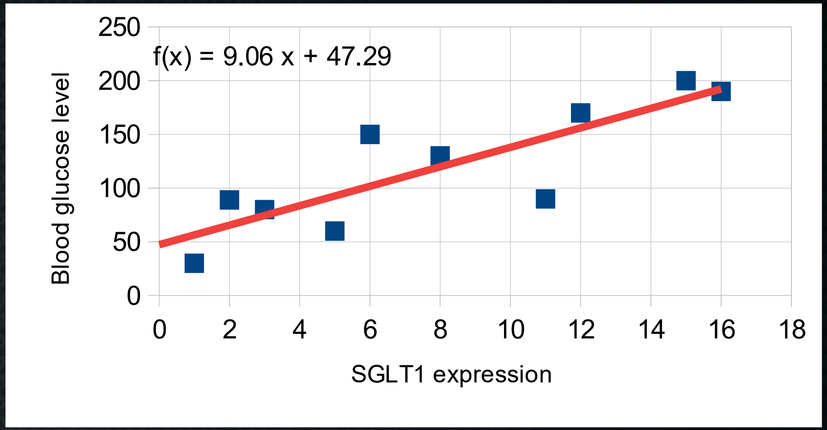
- How wrong are we for given parameters? $h_\theta(x)=\theta_0+\theta_1 x$



Cost function

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

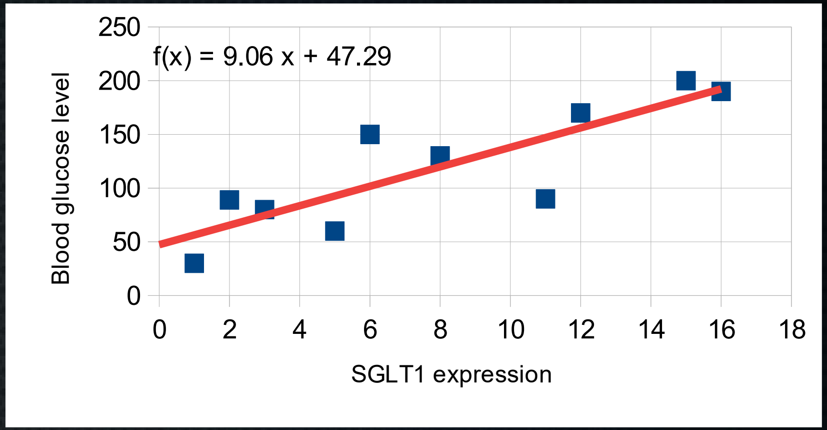
$$h_\theta(x)=\theta_0+\theta_1 x$$



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

Cost function

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



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

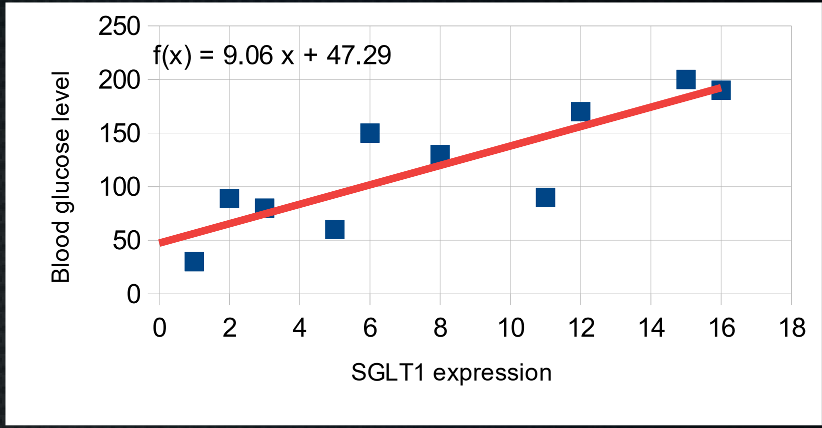
$$J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

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

Cost function

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

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



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

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

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

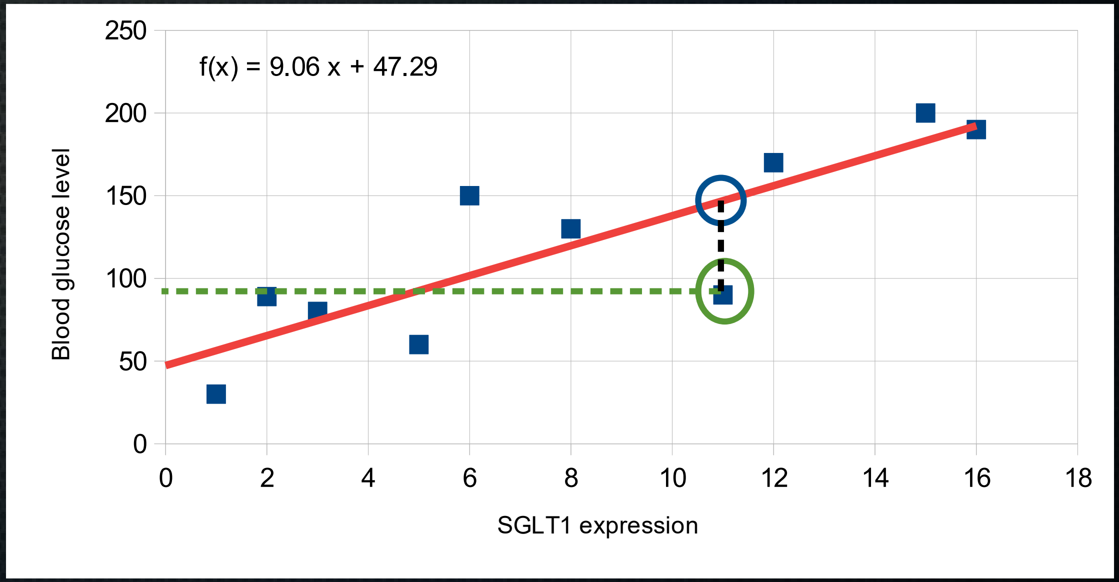
Cost function

- How wrong are we for given parameters? $h_\theta(x)=\theta_0+\theta_1 x$
- Cost function:

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

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

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



Cost function conclusion

$y = ax + b$

- If we want to be as correct as possible with our prediction, want to minimise:

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

Cost function conclusion

- If we want to be as correct as possible with our prediction, want to minimise:

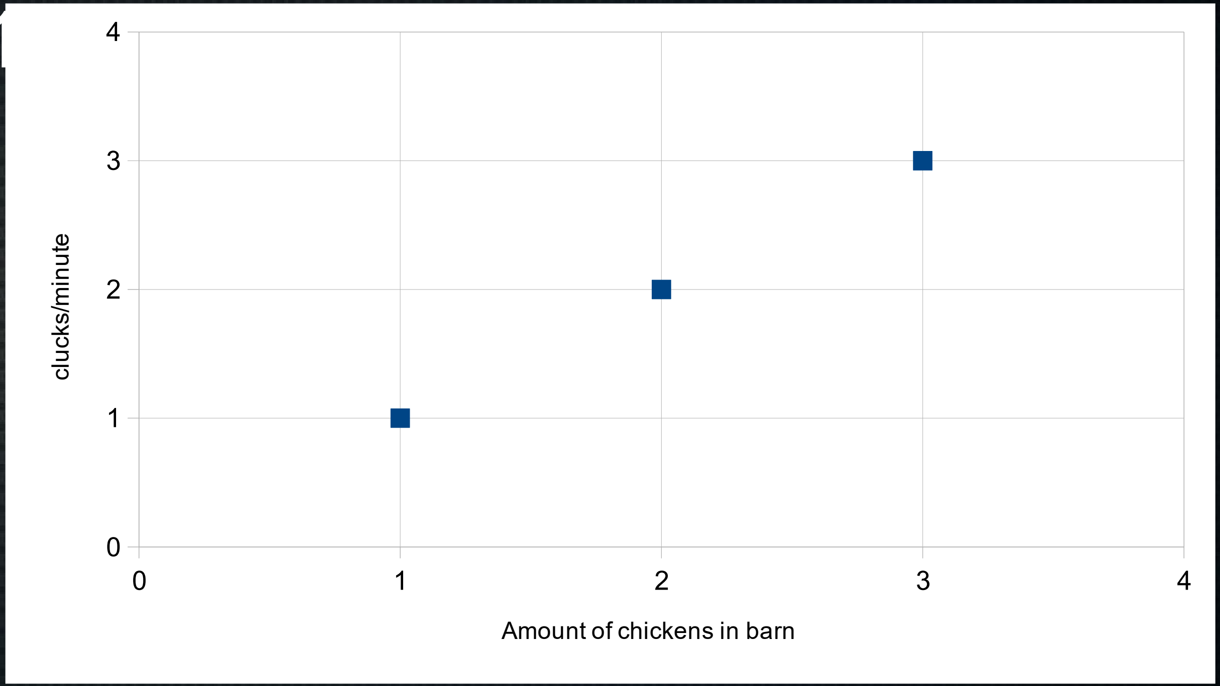
$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)})^2$$

- Simplified example: Theta0 = 0:

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

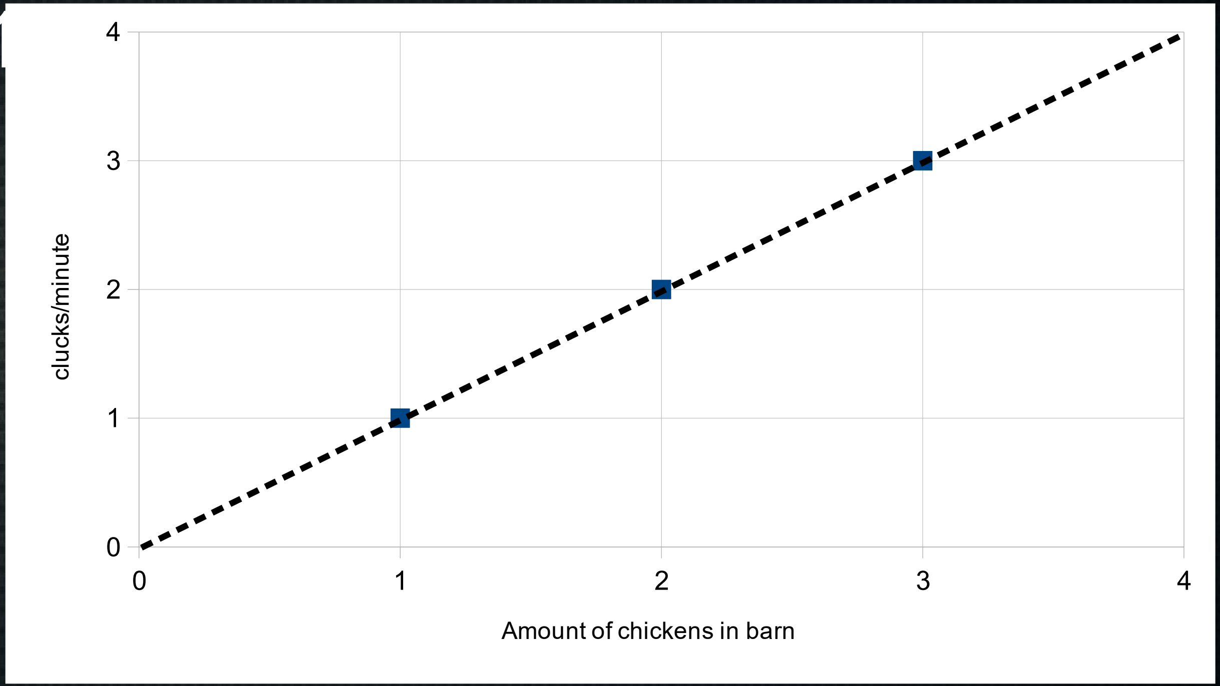
Cost function conclusion illustration

- Let's say theta0 = 0 (so the intercept is 0). What is J(theta1) for different values of theta1



Cost function illustration

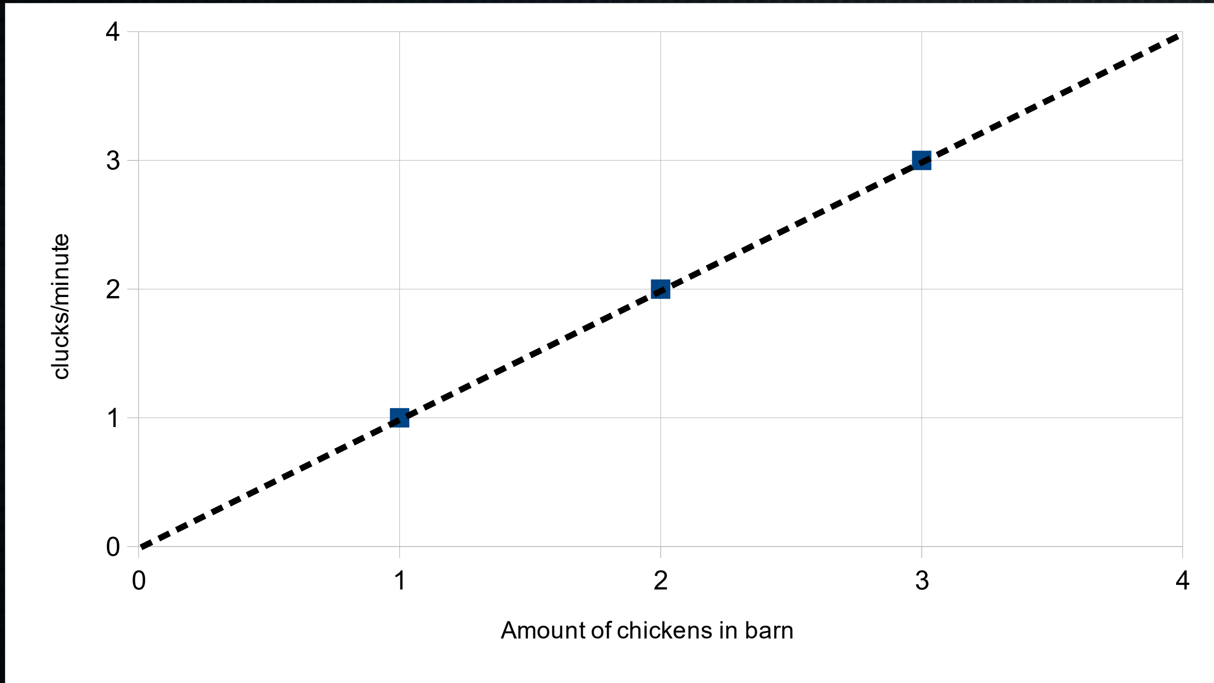
- Let‘s say theta0 = 0 (so the intercept is 0). What is J(theta1) for different values of theta1?
- Theta1 = 1

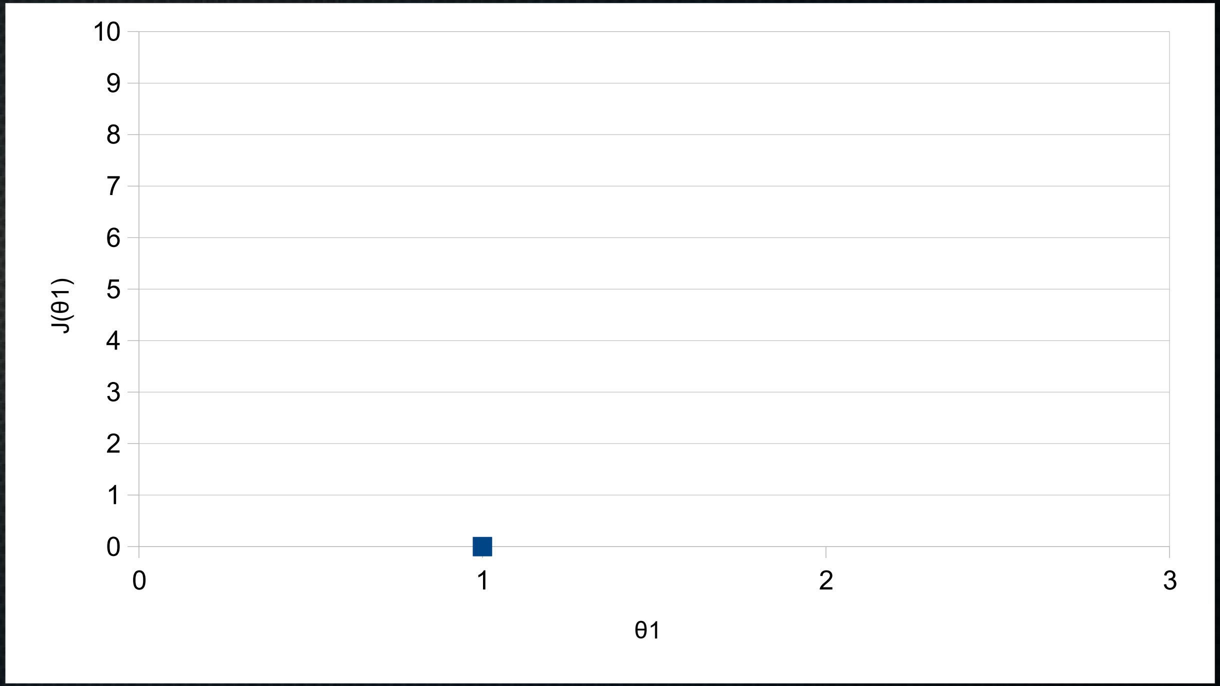


$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{3} (\theta_1 \cdot x^{(i)} - y^{(i)})^2$$

$$J(\theta_1) = 0$$

Cost function illustration

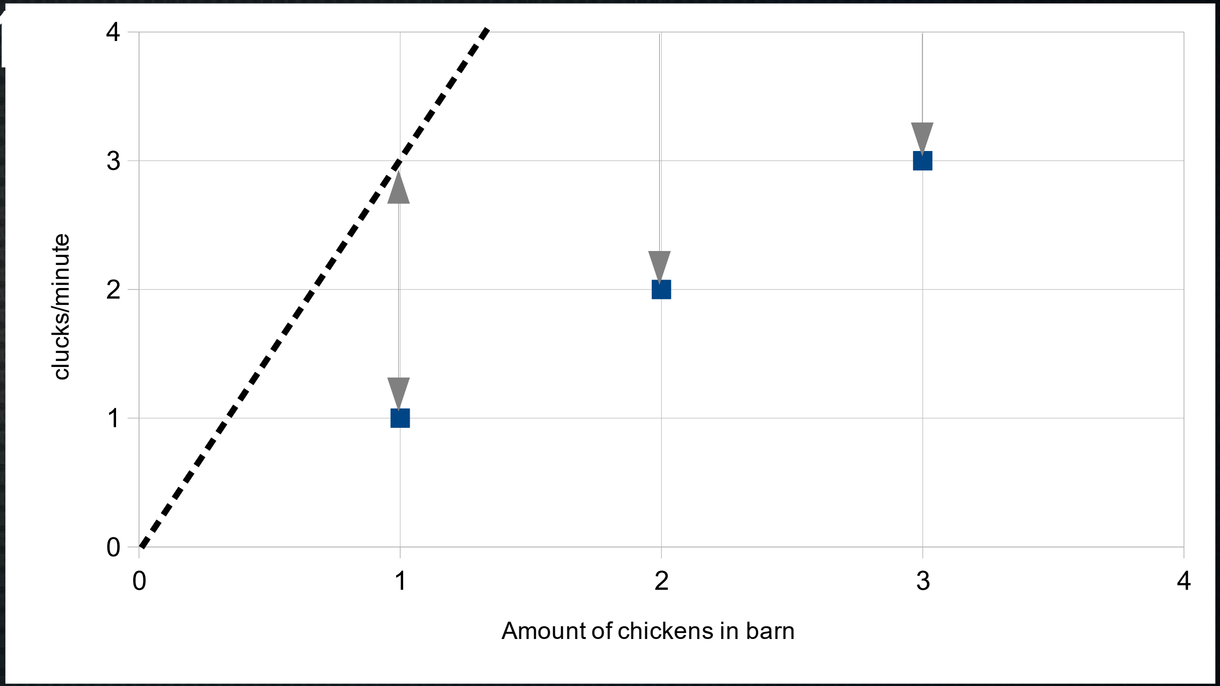




Cost function illustration

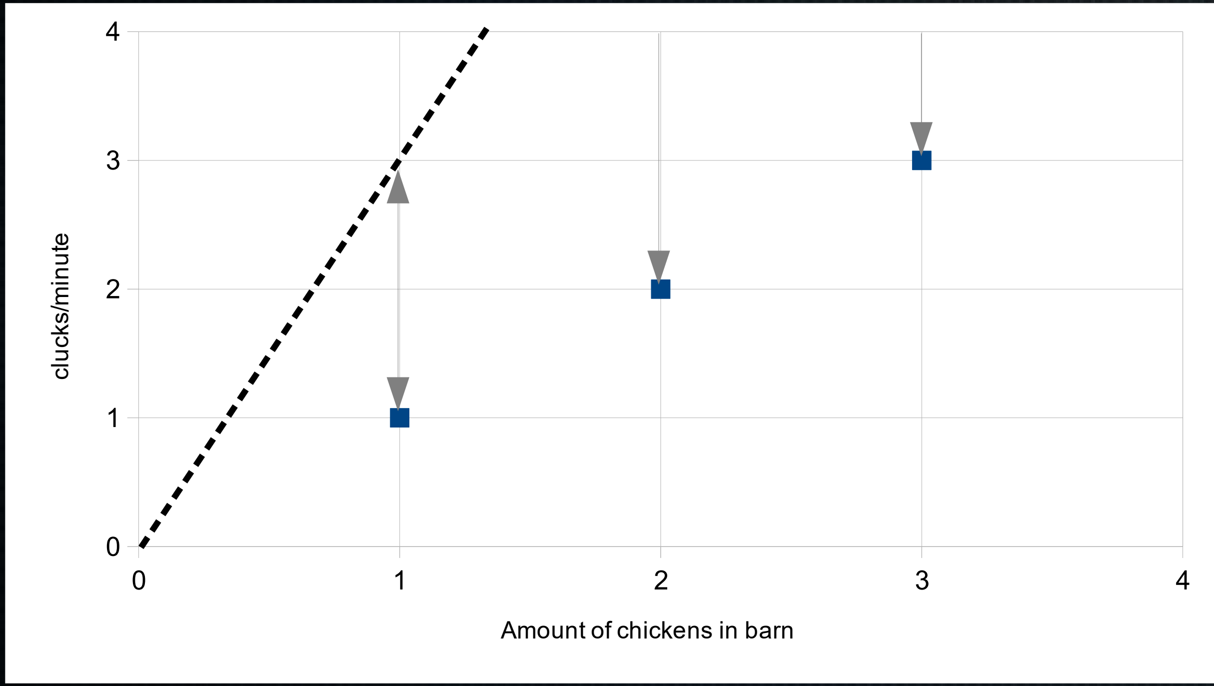
- Let‘s say theta0 = 0 (so the intercept is 0). What is J(theta1) for different values of theta1
- Theta1 = 3

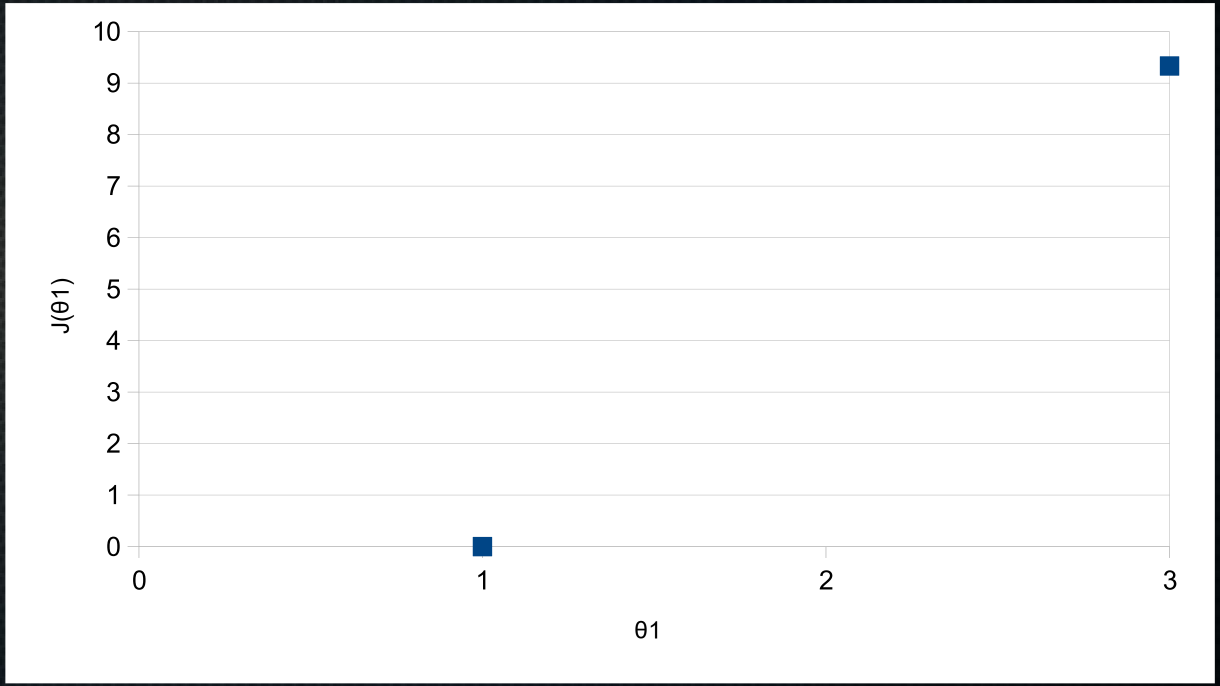
$$J(\theta_1)=\frac{1}{2m}\sum_{i=1}^{3}(\theta_1\cdot x^{(i)}-y^{(i)})^2$$



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

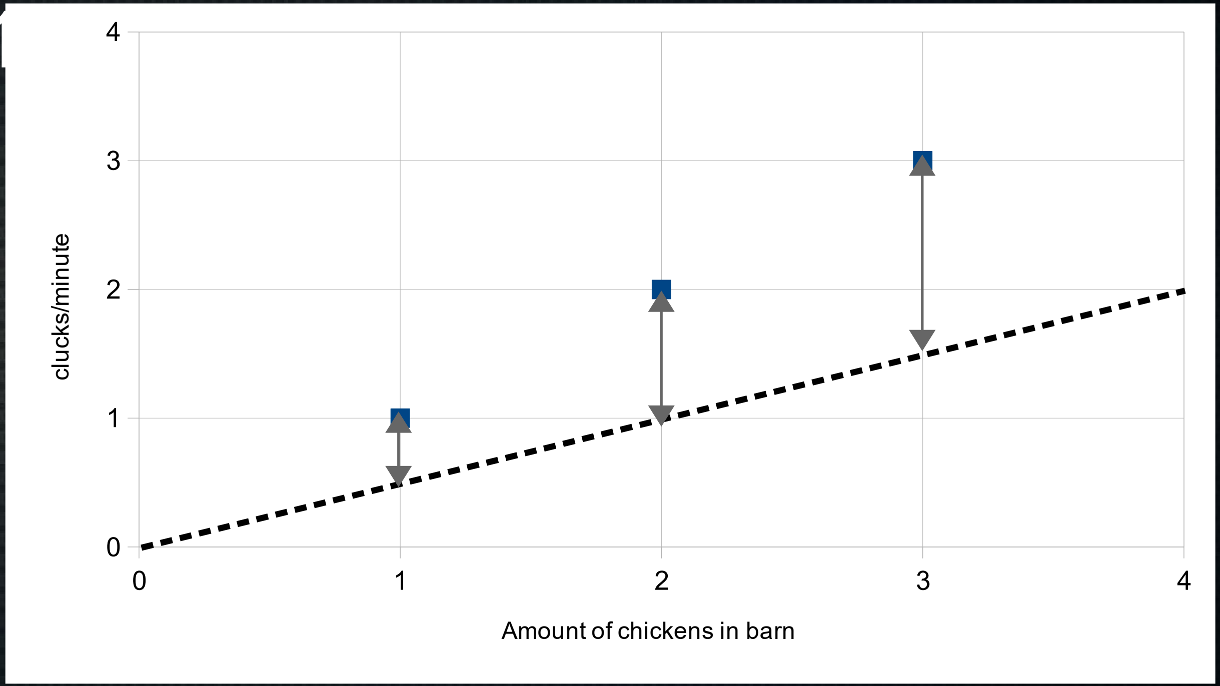
Cost function illustration





Cost function illustration

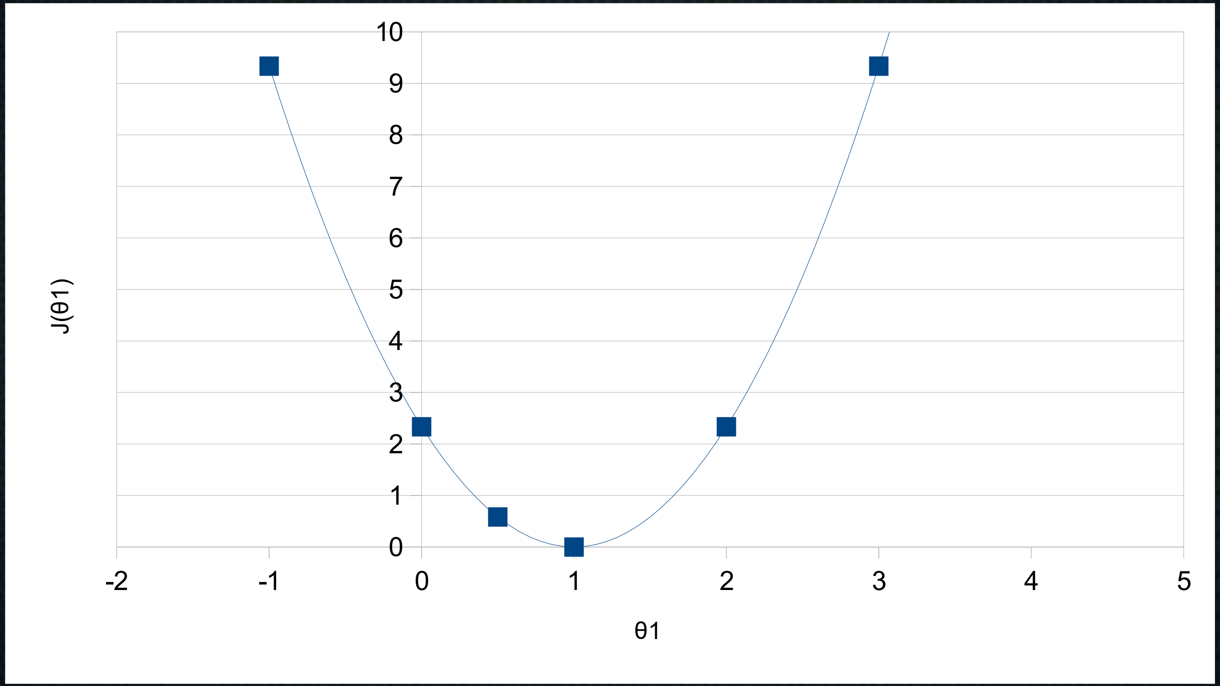
- Let‘s say theta0 = 0 (so the intercept is 0). What is J(theta1) for different values of theta1?
- Theta1 = 0.5



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

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

Cost function illustration

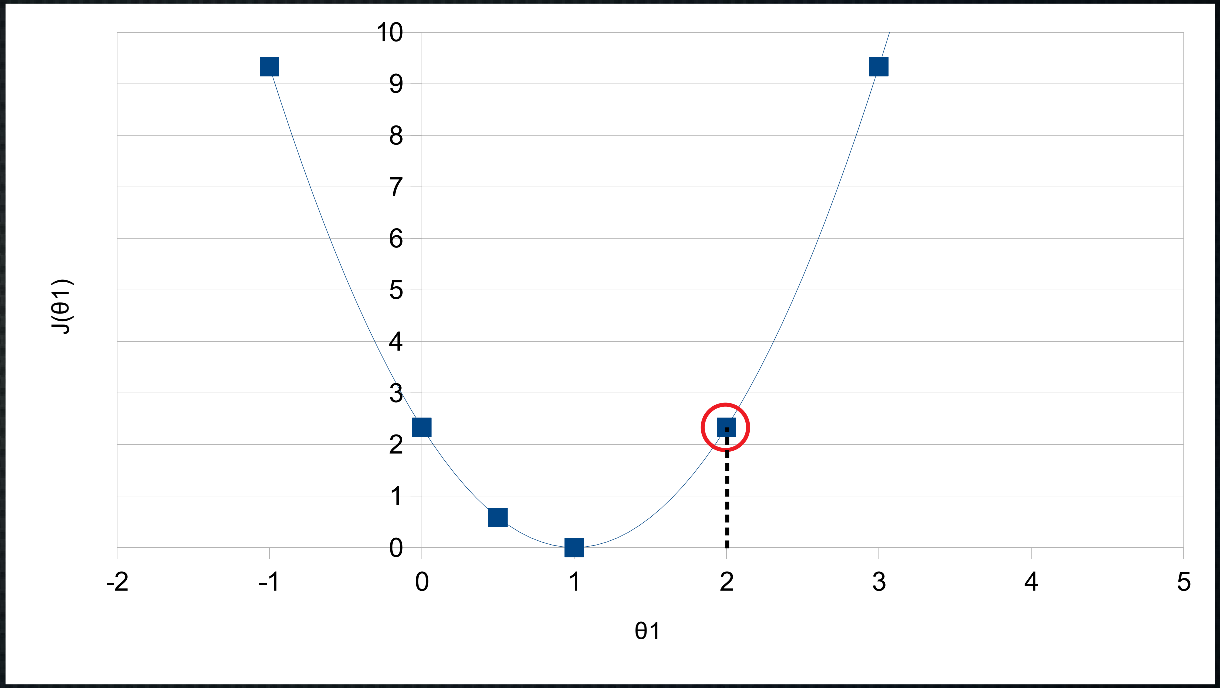


Cost function and gradient descent

- How to learn theta‘s from data?
- Two parts
  - How wrong are we for given parameters?
  - ***<u>How do we update our parameters, given how wrong we are?</u>***

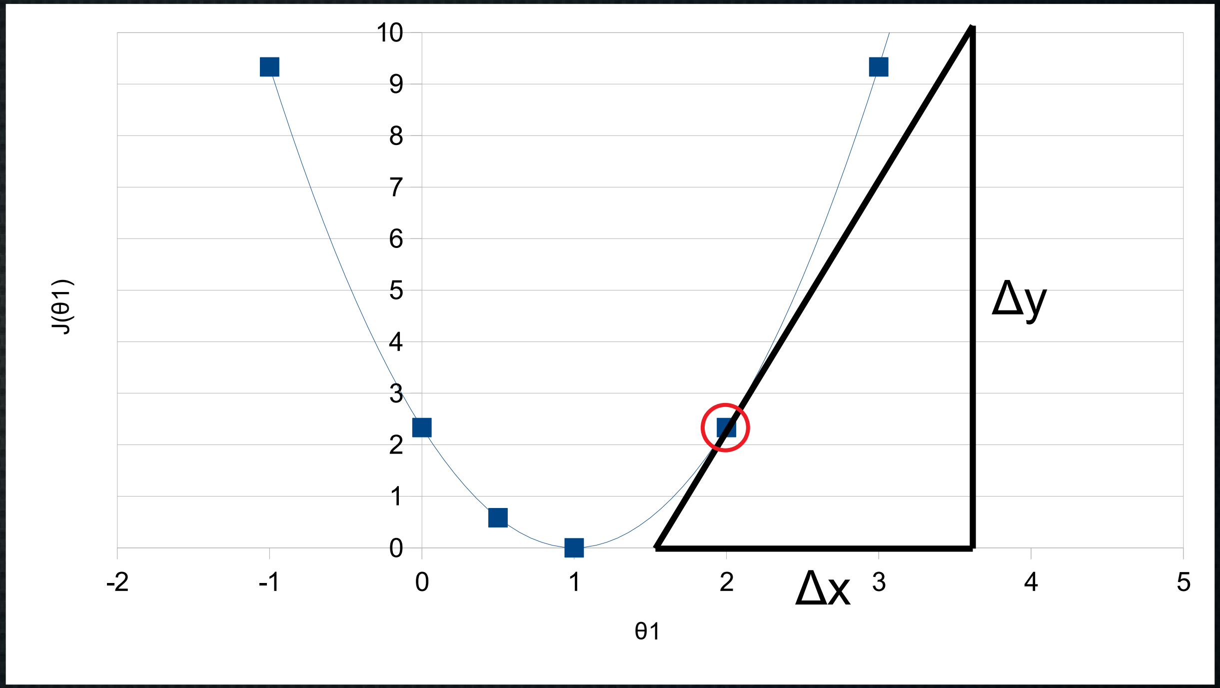
Gradient descent

- Want to minimise
- Where to go?



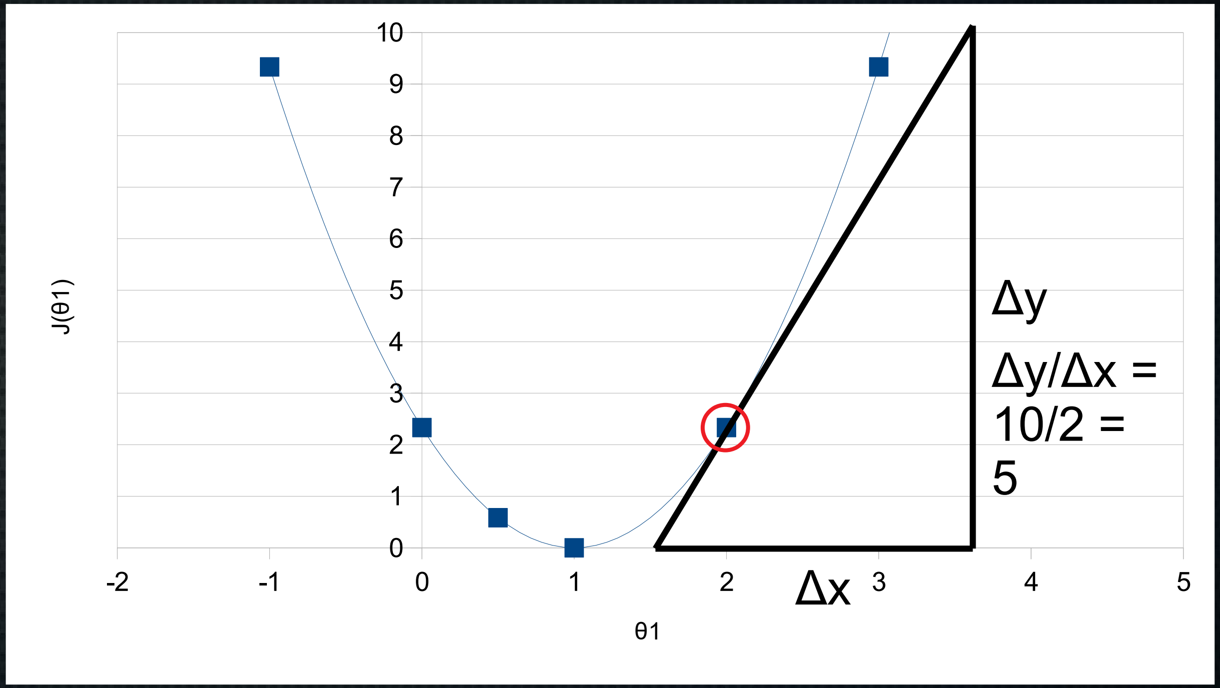
Gradient descent

- Want to minimise
- Where to go?



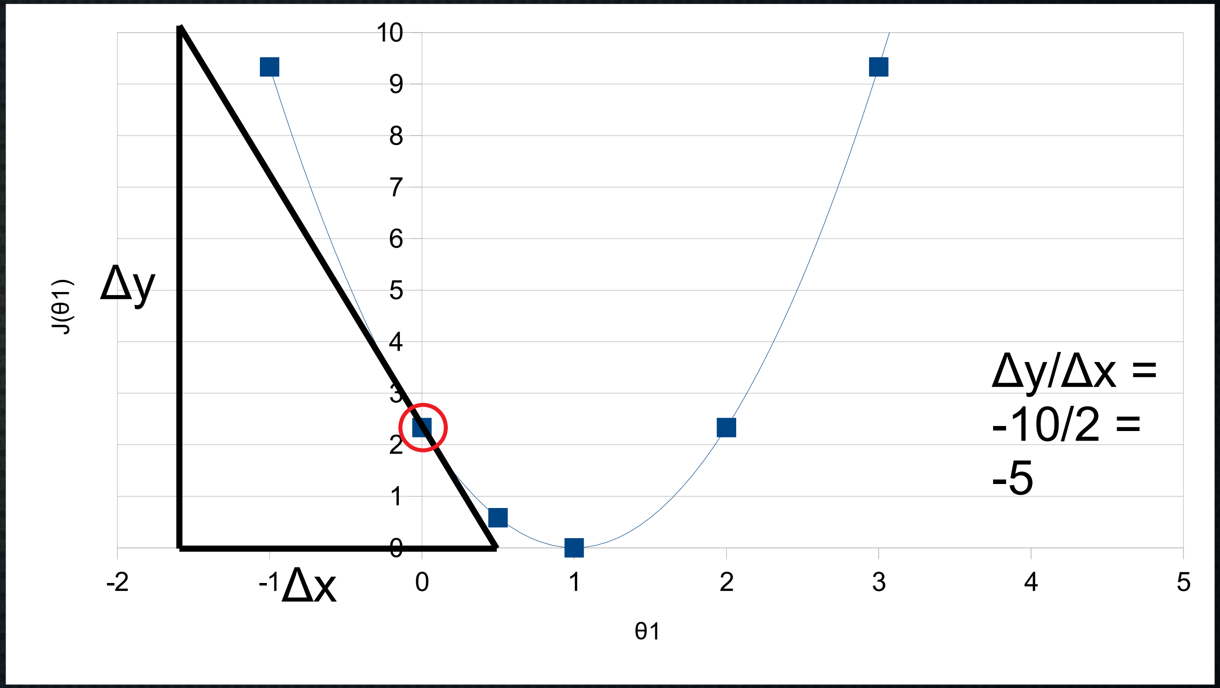
Gradient descent

- Want to minimise
- Where to go?



Gradient descent

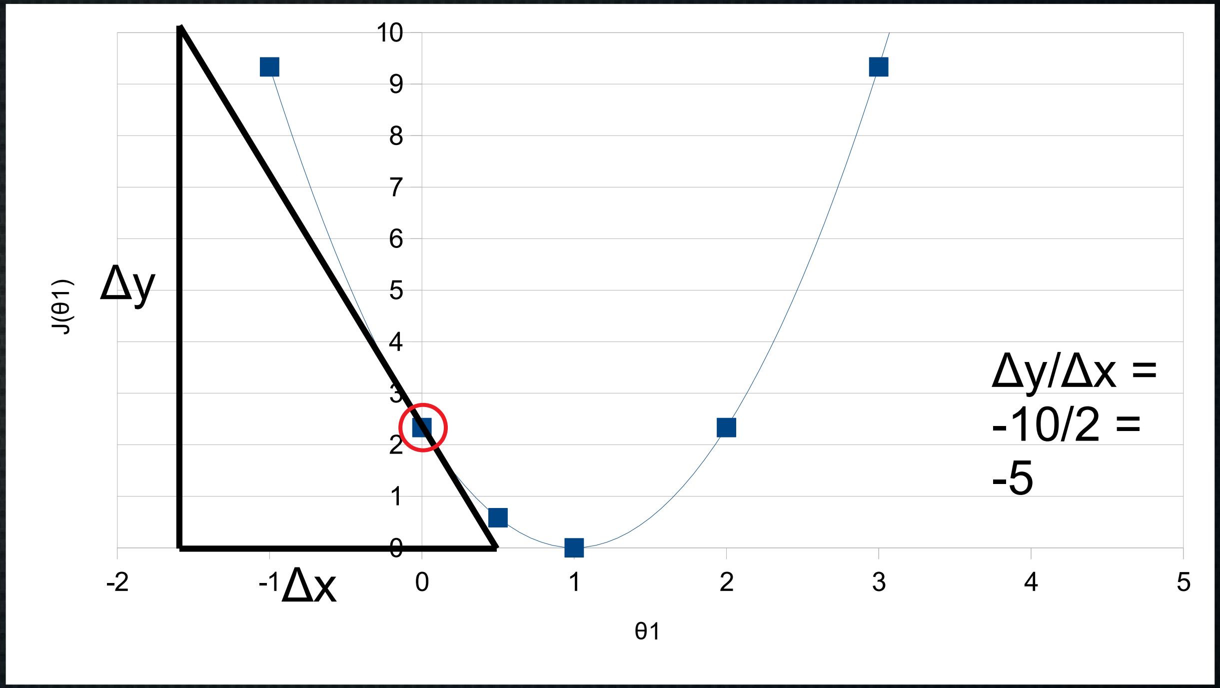
- Want to minimise
- Where to go?



Gradient descent

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

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



Gradient descent

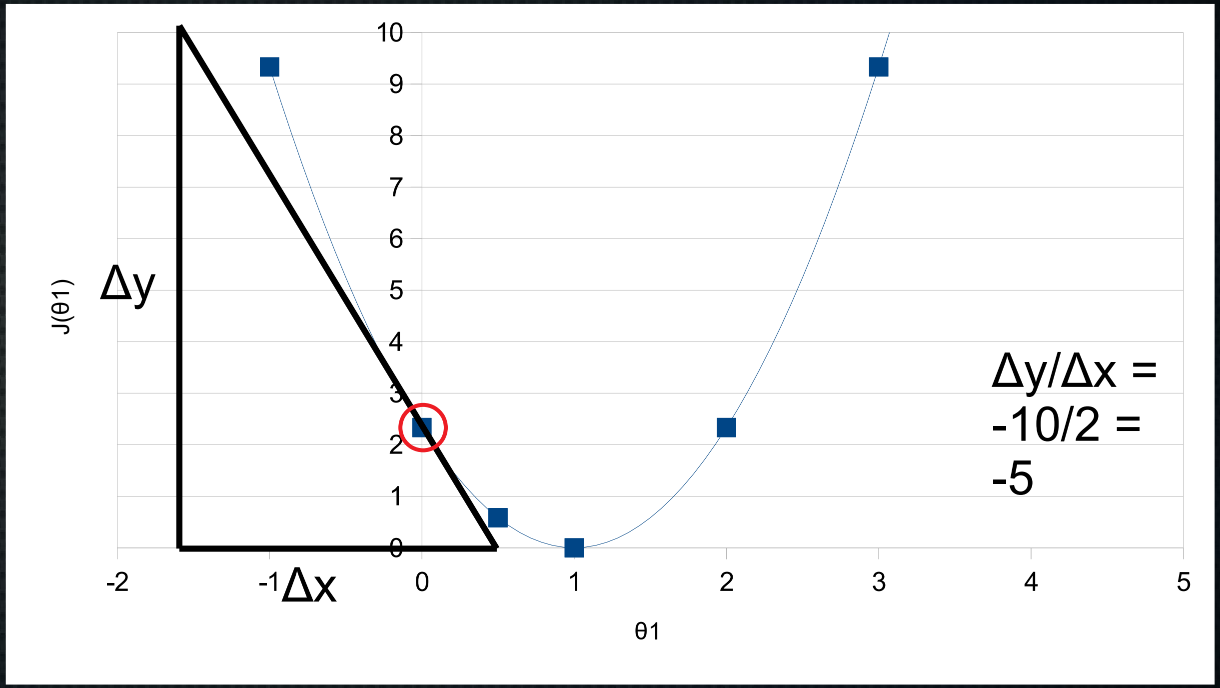
- Want to minimise
- Where to go?
- Change current theta1 as follows:

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

$$\alpha = 0.2$$

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

$$\theta_1 = 1$$



Gradient descent

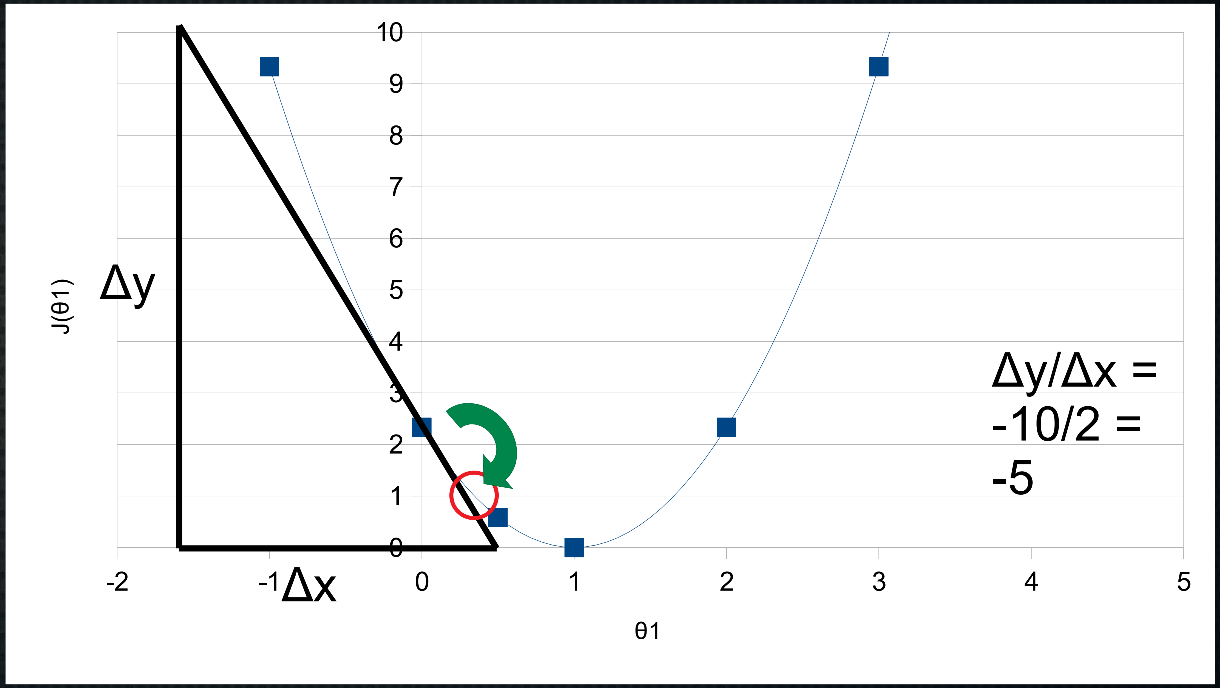
- Want to minimise
- Where to go?
- Change current theta1 as follows:

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

$$\alpha = 0.2$$

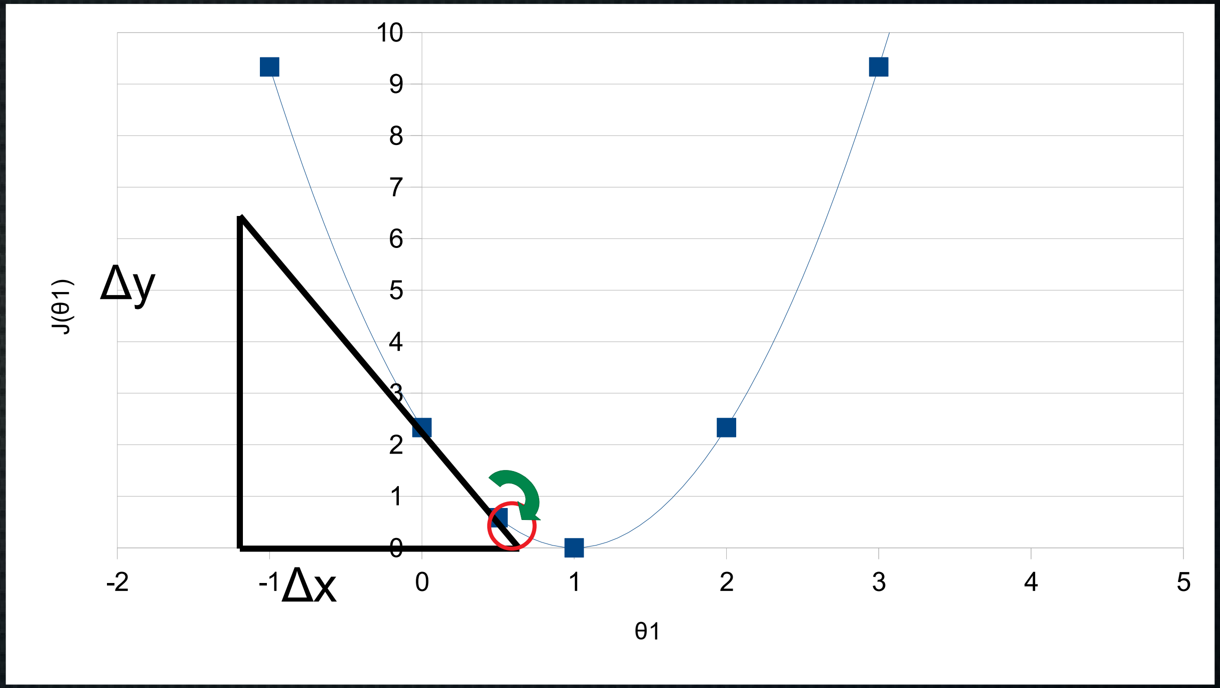
$$\theta_1 = 0 - 0.2 \cdot -5$$

$$\theta_1 = 1$$



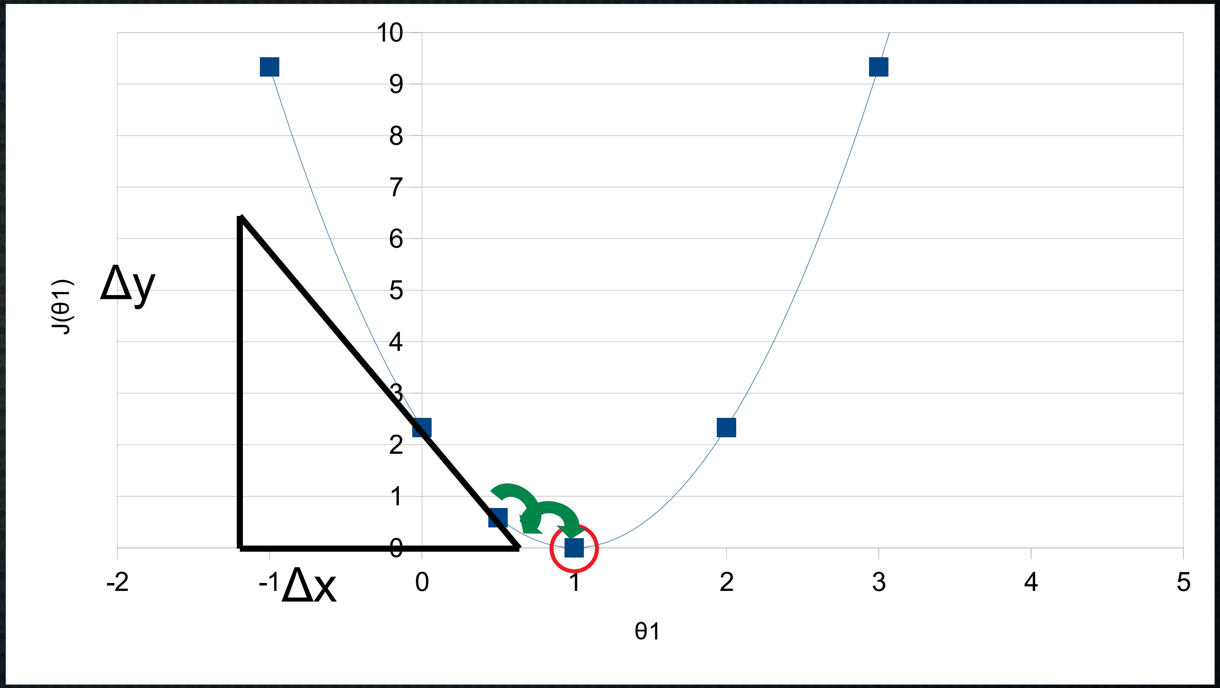
Gradient descent

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



Gradient descent

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



Gradient descent

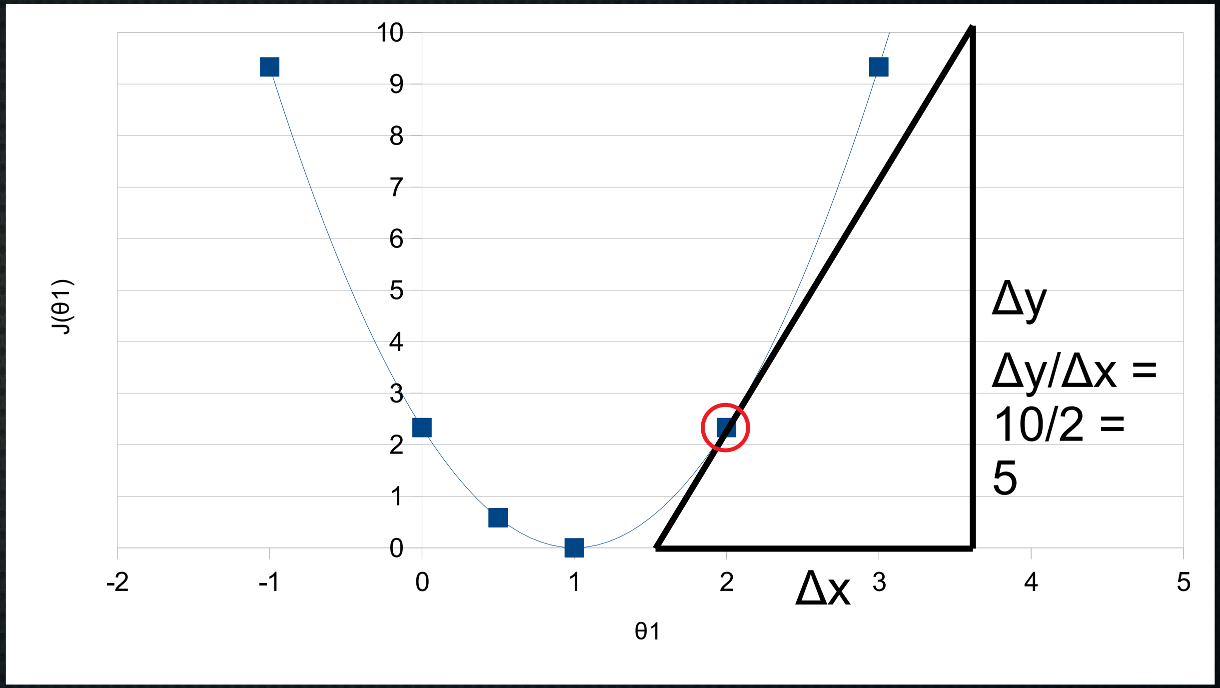
- Works also from other direction.

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

$$\alpha = 0.2$$

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

$$\theta_1 = 1$$

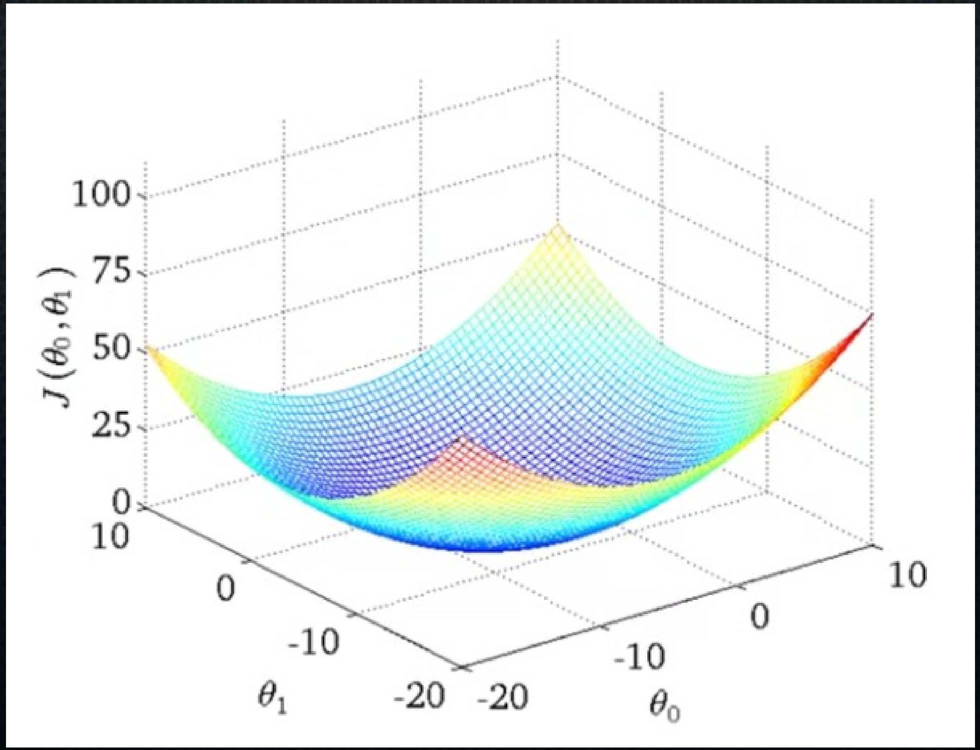


Gradient descent

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

Gradient descent

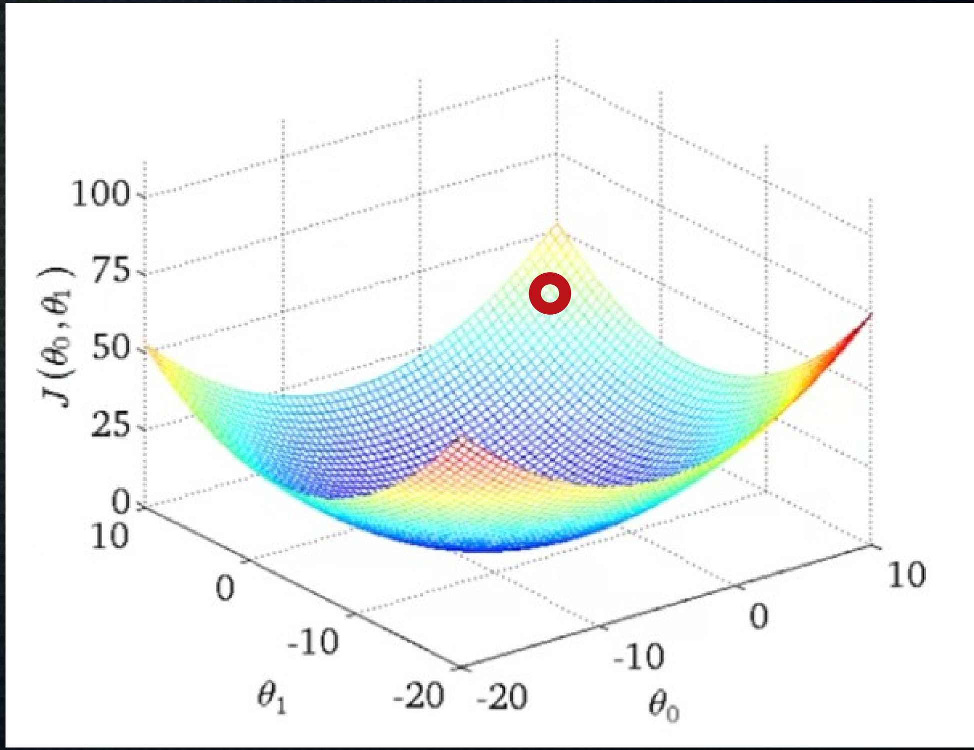
- Iteratively descend down the gradient of the cost function until convergence → optimal parameters!
- In reality: not one-dimensional:



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

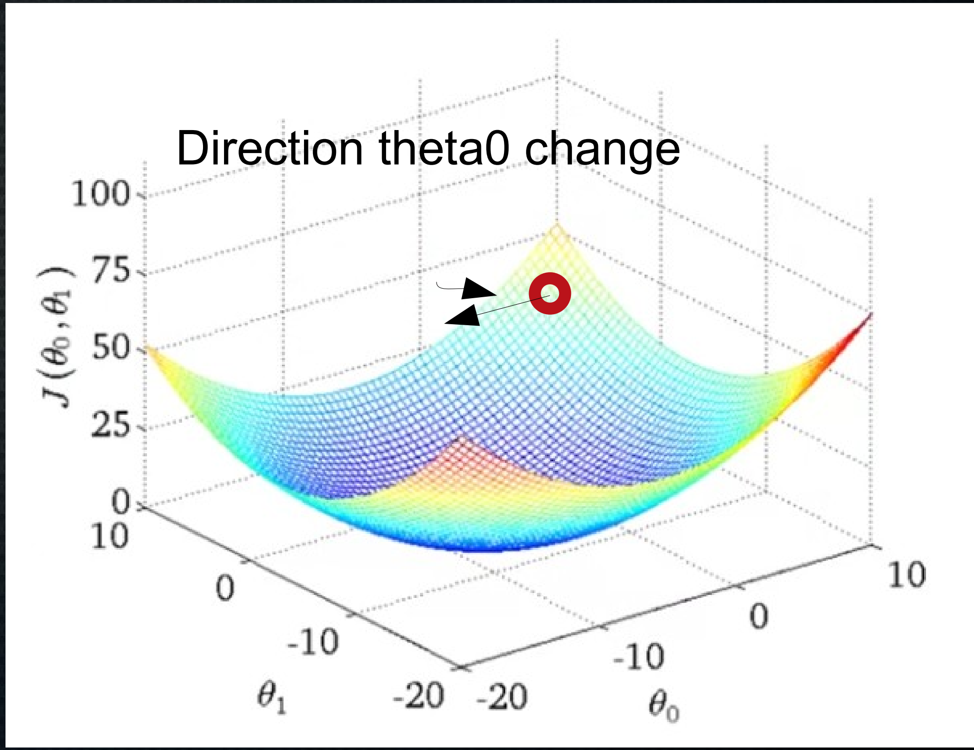
- Iteratively descend down the gradient of the cost function until convergence → optimal parameters!
- In reality: not one-dimensional.
  Want to fit intercept *and* slope.
- Use partial derivatives instead:



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

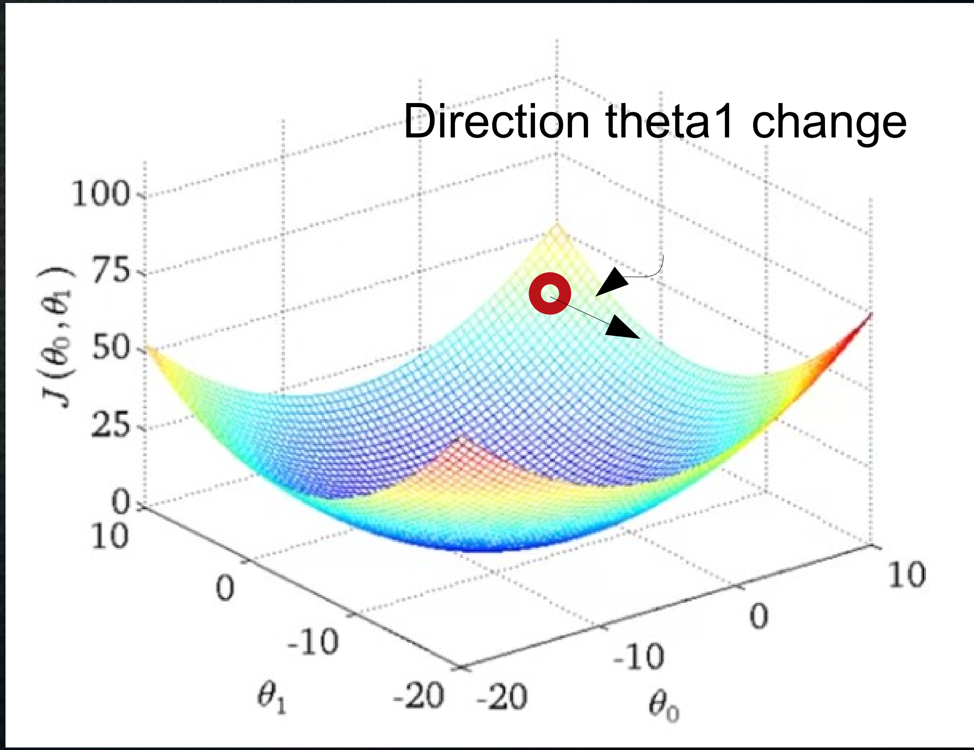
- Iteratively descend down the gradient of the cost function until convergence → optimal parameters!
- In reality: not one-dimensional. Want to fit intercept *and* slope.
- Use partial derivatives instead:



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

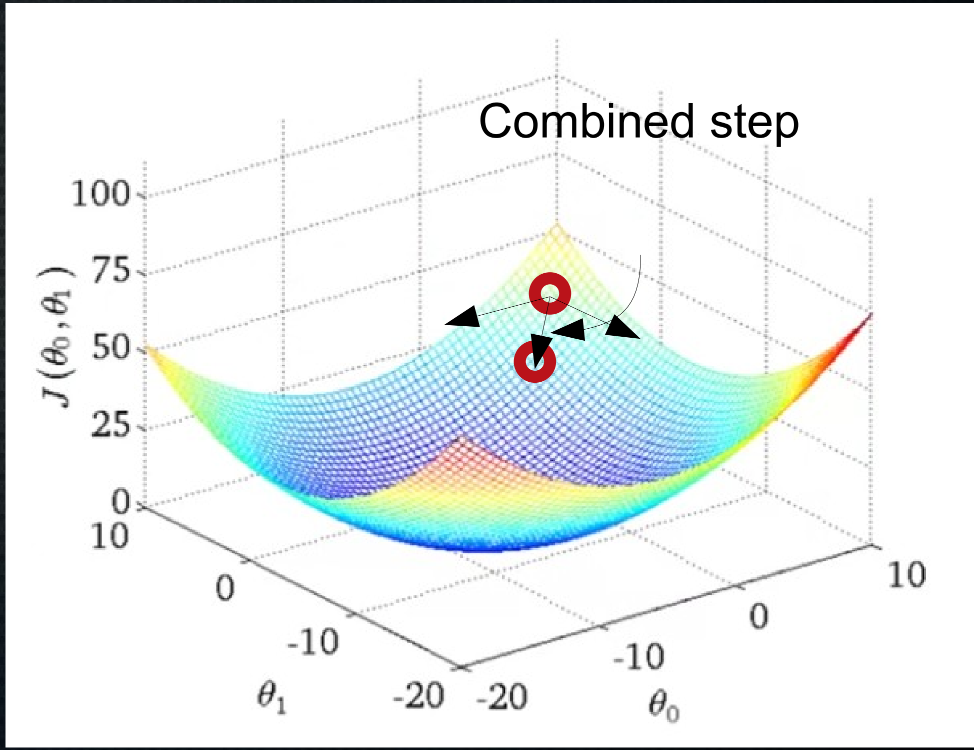
- Iteratively descend down the gradient of the cost function until convergence → optimal parameters!
- In reality: not one-dimensional.
  Want to fit intercept *and* slope.
- Use partial derivatives instead:



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

- 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:

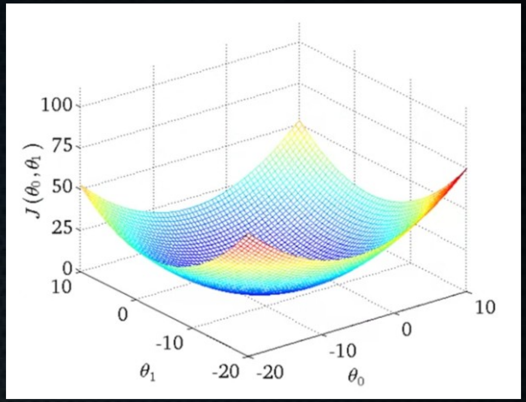


Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

- Partial derivatives:

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



Source: Andrew Ng, Coursera

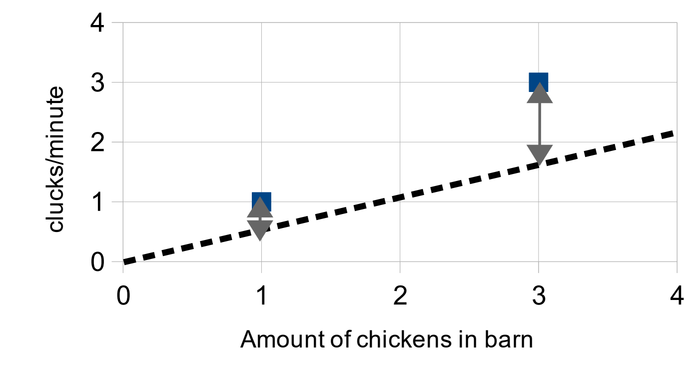
Gradient descent: partial derivatives

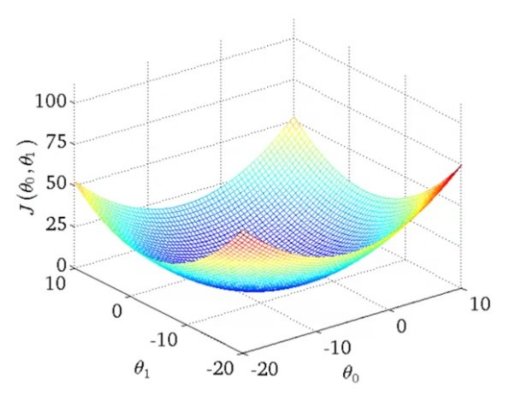
- Partial derivatives:

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

$$m=2$$

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





Source: Andrew Ng, Coursera

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

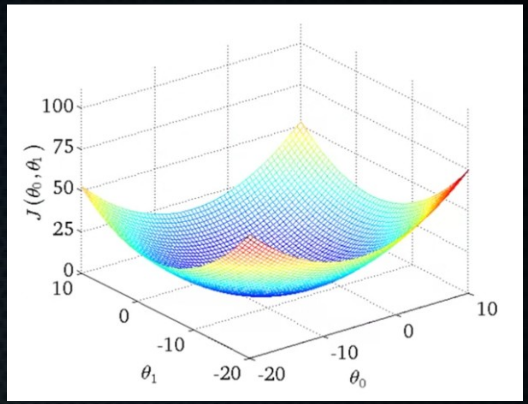
Gradient descent: partial derivatives

- Partial derivatives:

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

$$m = 2$$

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



Source: Andrew Ng, Coursera

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

Gradient descent: partial derivatives

- Partial derivatives:

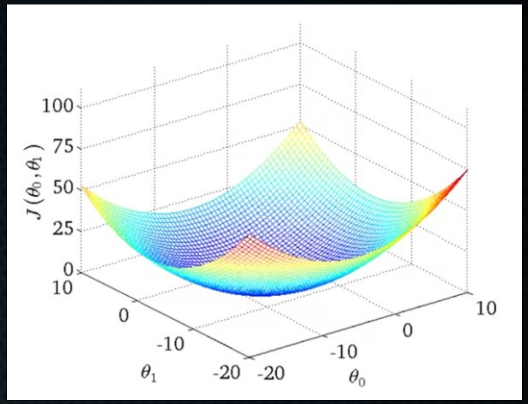
$$J(\theta_0,\theta_1)=\frac{1}{2m}\sum_{i=1}^{m}(\theta_0+\theta_1\cdot x^{(i)}-y^{(i)})^2$$

$$m=2$$

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

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

$$+\underline{2(\theta_0+\theta_1\cdot x^{(2)}-y^{(2)})}*1)$$

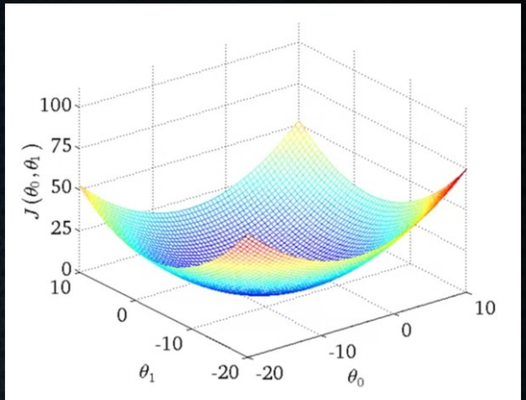


Source: Andrew Ng, Coursera

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

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

Gradient descent: partial derivatives



Source: Andrew Ng, Coursera

- Partial derivatives:

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

$$m=2$$

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

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

$$\left.+\underline{2\left(\theta_0+\theta_1\cdot x^{(2)}-y^{(2)}\right)}*\underline{1}\right)$$

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

Gradient descent: partial derivatives

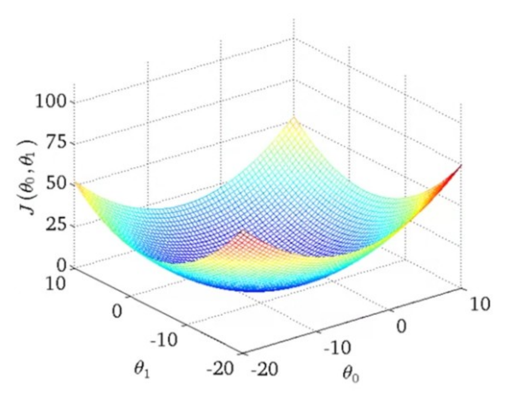
- Partial derivatives:

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

$$m=2$$

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

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



Source: Andrew Ng, Coursera

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

Gradient descent: partial derivatives

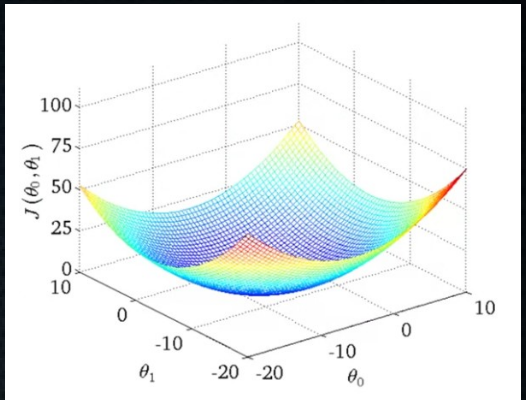
- Partial derivatives:

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

$$m=2$$

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

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



Source: Andrew Ng, Coursera

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

Gradient descent: partial derivatives

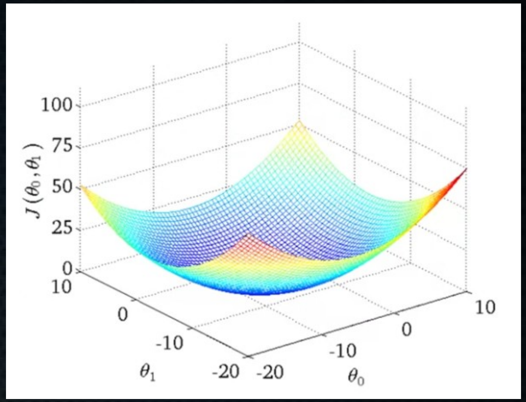
- Partial derivatives:

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

$$m=2$$

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

$$+2(\theta_0+\theta_1\cdot x^{(2)}-y^{(2)})*1)$$



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

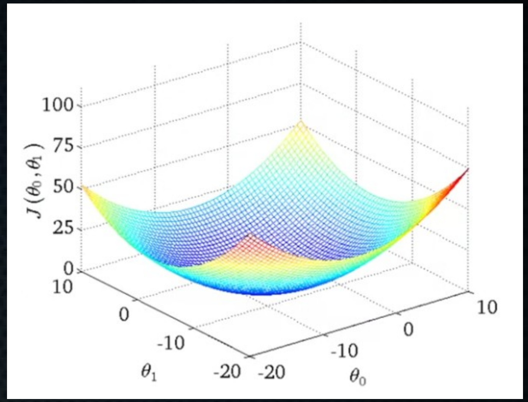
- Partial derivatives:

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

$$m = 2$$

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

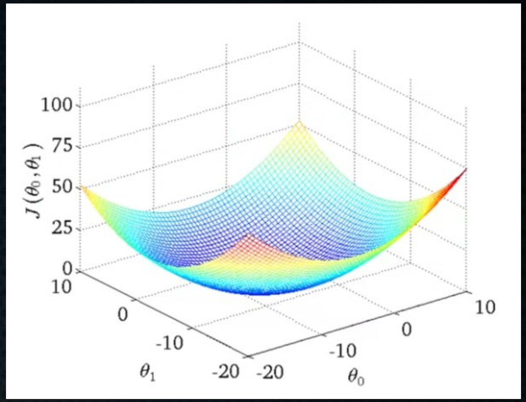
$$+ \underline{2} \underbrace{(\theta_0 + \theta_1 \cdot x^{(2)} - y^{(2)}) * 1} \Big)$$



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives

- Partial derivatives:



Source: Andrew Ng, Coursera

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

$$m = 2$$

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

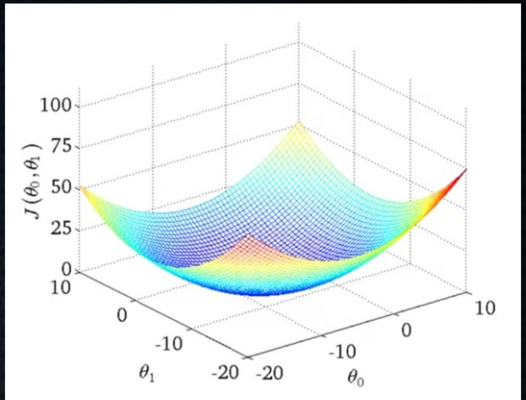
Gradient descent: partial derivatives

- Partial derivatives:

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

$$m=2$$

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



Source: Andrew Ng, Coursera

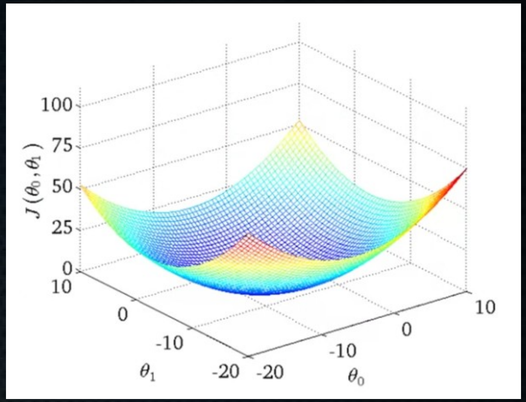
Gradient descent: partial derivatives

- Partial derivatives:

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

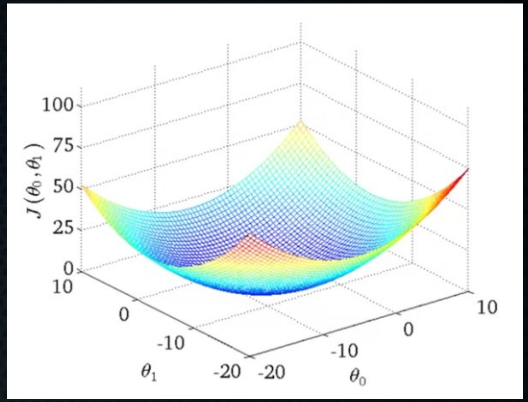
$$m = 2$$

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



Source: Andrew Ng, Coursera

Gradient descent: partial derivatives



Source: Andrew Ng, Coursera

- Partial derivatives:

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

$$m = 2$$

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

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

Gradient descent: partial derivatives

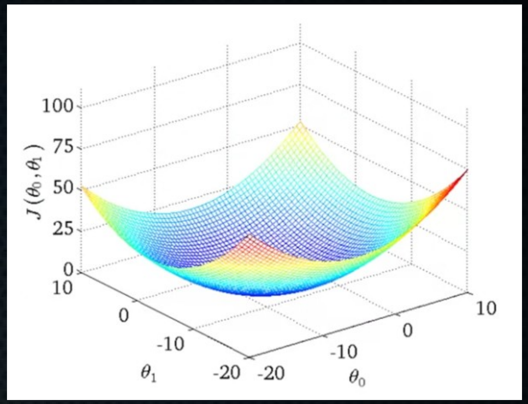
- Partial derivatives:

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

$$m = 2$$

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

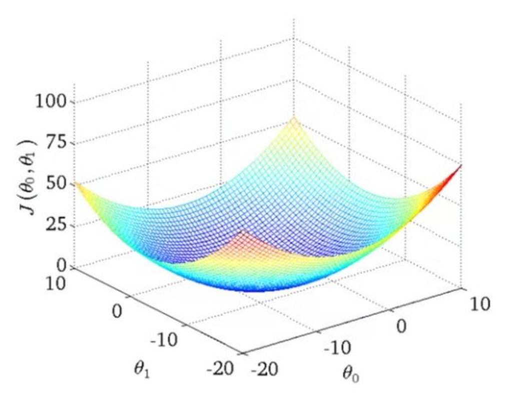
$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} (\theta_0 + \theta_1 \cdot x^{(i)} - y^{(i)}) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})$$



Source: Andrew Ng, Coursera

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

Gradient descent: partial derivatives



Source: Andrew Ng, Coursera

- Partial derivatives:

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

$$m=2$$

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

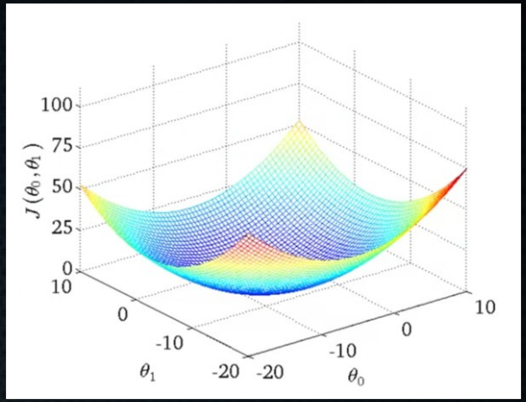
$$\frac{\partial}{\partial\theta_1}J(\theta_0,\theta_1)=\frac{1}{2\cdot 2}\Big(2\left(\theta_0+\theta_1\cdot x^{(1)}-y^{(1)}\right)*\underline{x^{(1)}}$$
$$+2\left(\theta_0+\theta_1\cdot x^{(2)}-y^{(2)}\right)*\underline{x^{(2)}}\Big)$$

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

Gradient descent: partial derivatives

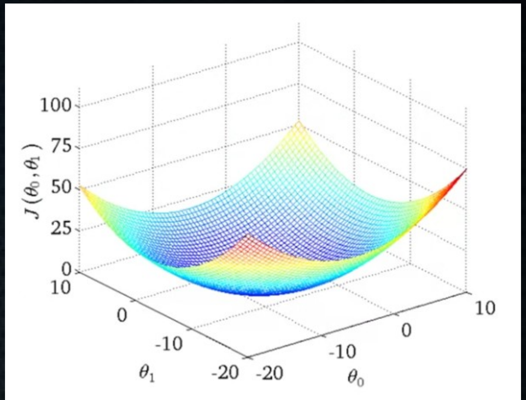
- Partial derivative theta1:

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



Source: Andrew Ng, Coursera

Cost function and gradient descent



Source: Andrew Ng, Coursera

- Cost function:

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

- Partial derivatives for gradient descent:

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

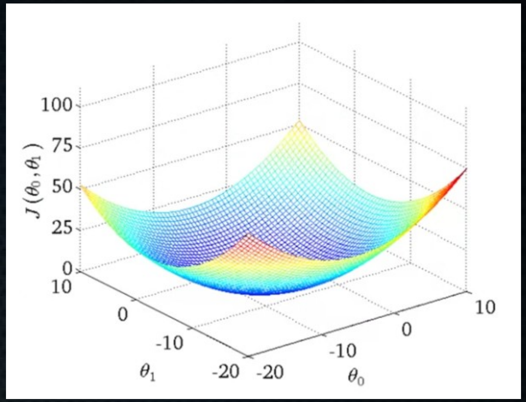
$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(\left(h_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}\right)$$

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

Cost function and gradient descent

- Cost function:

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



Source: Andrew Ng, Coursera

- Gradient descent update:

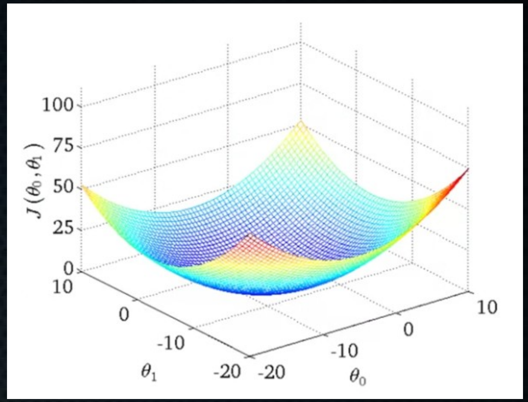
$$\theta_0=\theta_0-\alpha\frac{\partial}{\partial\theta_0}J(\theta_0,\theta_1)=\theta_0-\frac{\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})$$

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

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

What about α?

- Learning rate, so-called hyperparameter.

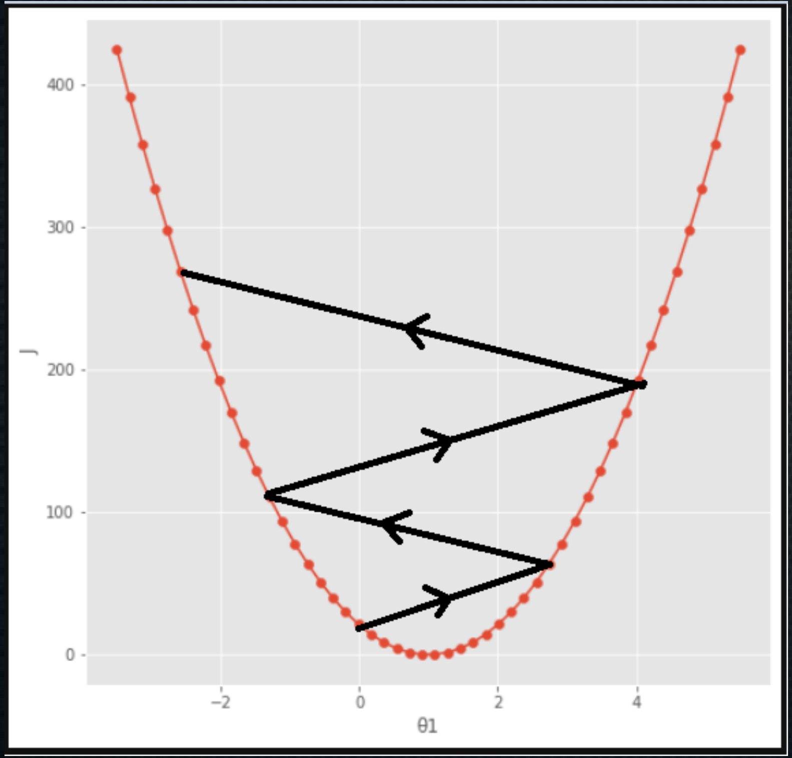


Source: Andrew Ng, Coursera

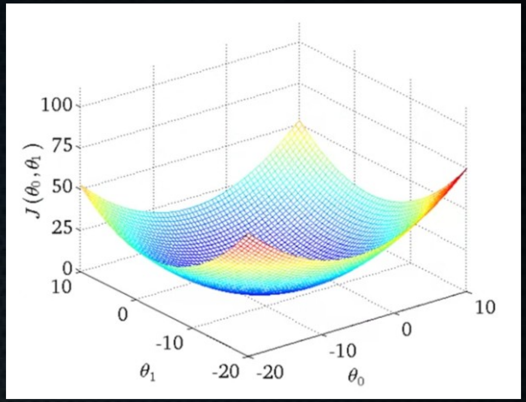
$$\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)$$

What about α?

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



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

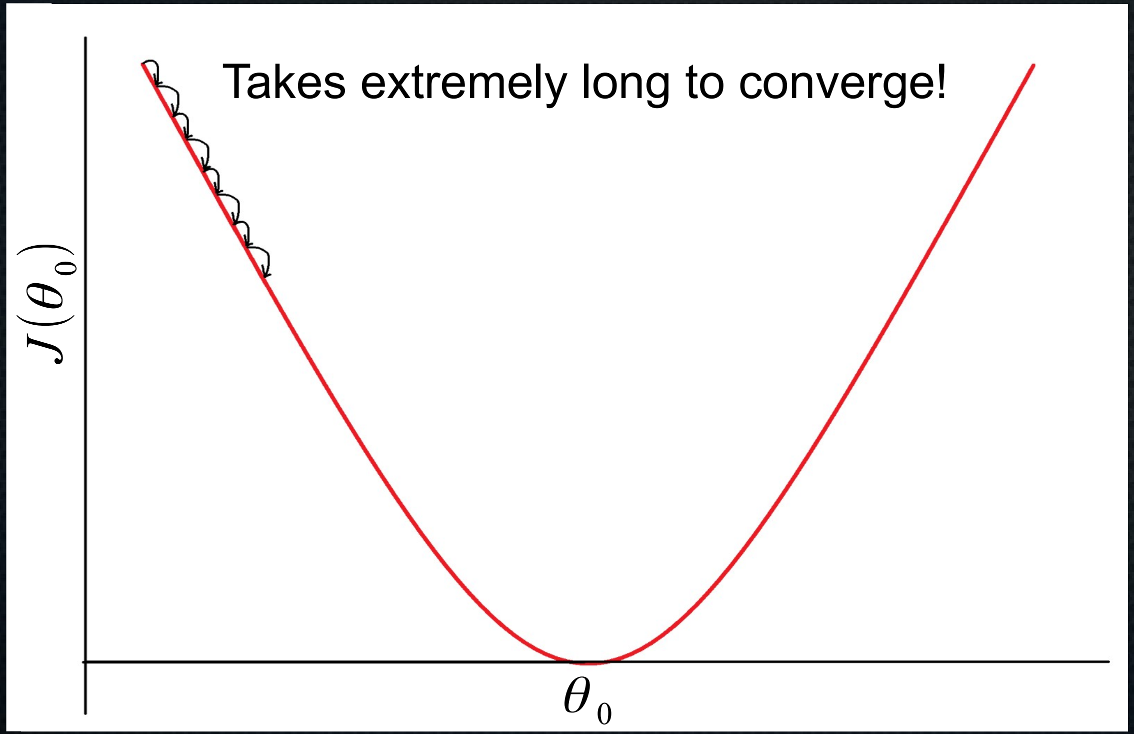


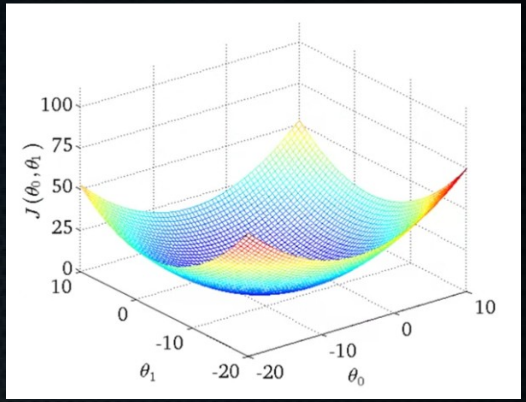
Source: Andrew Ng, Coursera

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

What about α?

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



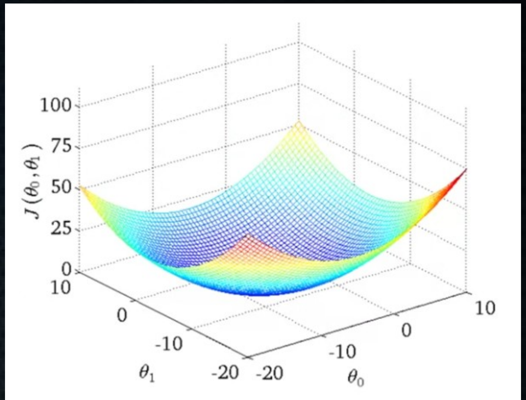


Source: Andrew Ng, Coursera

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

What about α?

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



Source: Andrew Ng, Coursera

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

Practicals

- You should now open and do *Day1/Practical/PracticalMaterialDay1_ShortPractical1.ipynb*
- Open Anaconda prompt, navigate to *Basic-Machine-Learning-for-Bioinformatics*, and type *jupyter notebook.* Then navigate to and open the correct file in this browser interface.
- DuckDuckGo and Google are your friend: numpy takes some getting used to, so search, search, search!
- I will start the next lecture in about an hour. If you're not finished: don't worry! Just continue where you left off after the lecture.