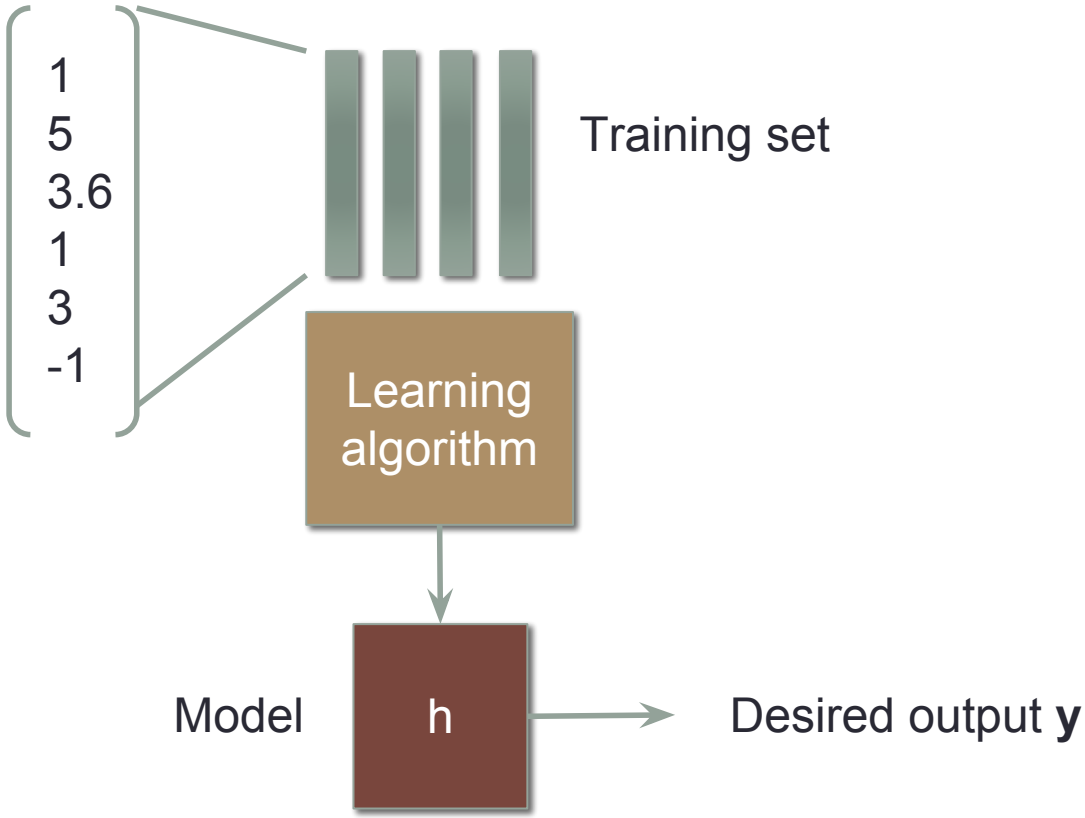
# REGRESSION

with some K-mean clustering

# How do we learn from data?




Training phase

# Types of machine learning

1. Supervised learning

   Learn a model F from pairs of (**x**,y)

2. Unsupervised learning

   Discover the hidden structure in unlabeled data **x** (no y)

3. Reinforcement learning

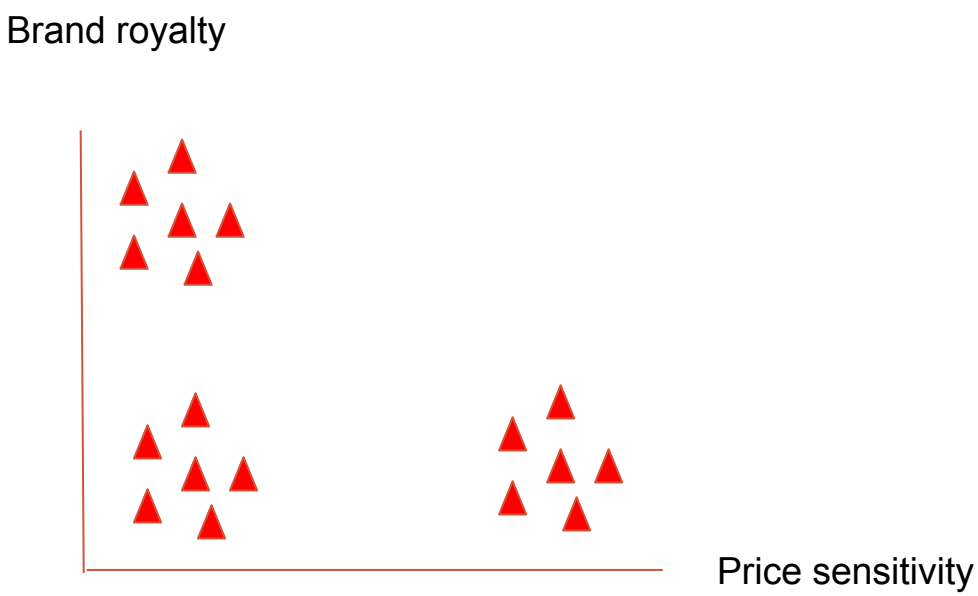
   Train an agent to take appropriate actions in an environment by maximizing rewards

# Our first model - Unsupervised learning

Discover the hidden structure in unlabeled data X (no y)

- Customer/product segmentation
- Data analysis for ...
- Identify number of speakers in a meeting recording
- Helps supervised learning in some task

# Example - Customer analysis



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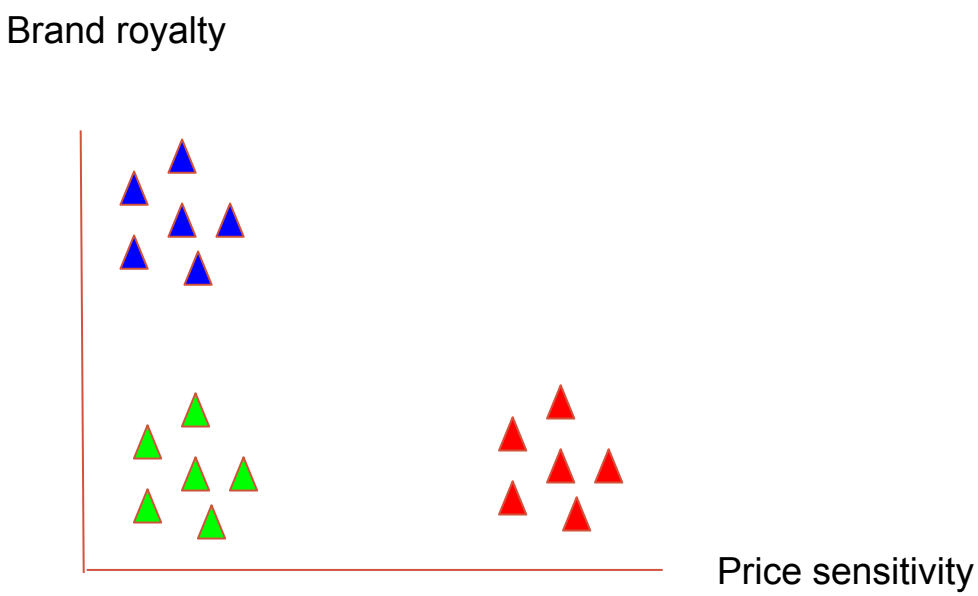
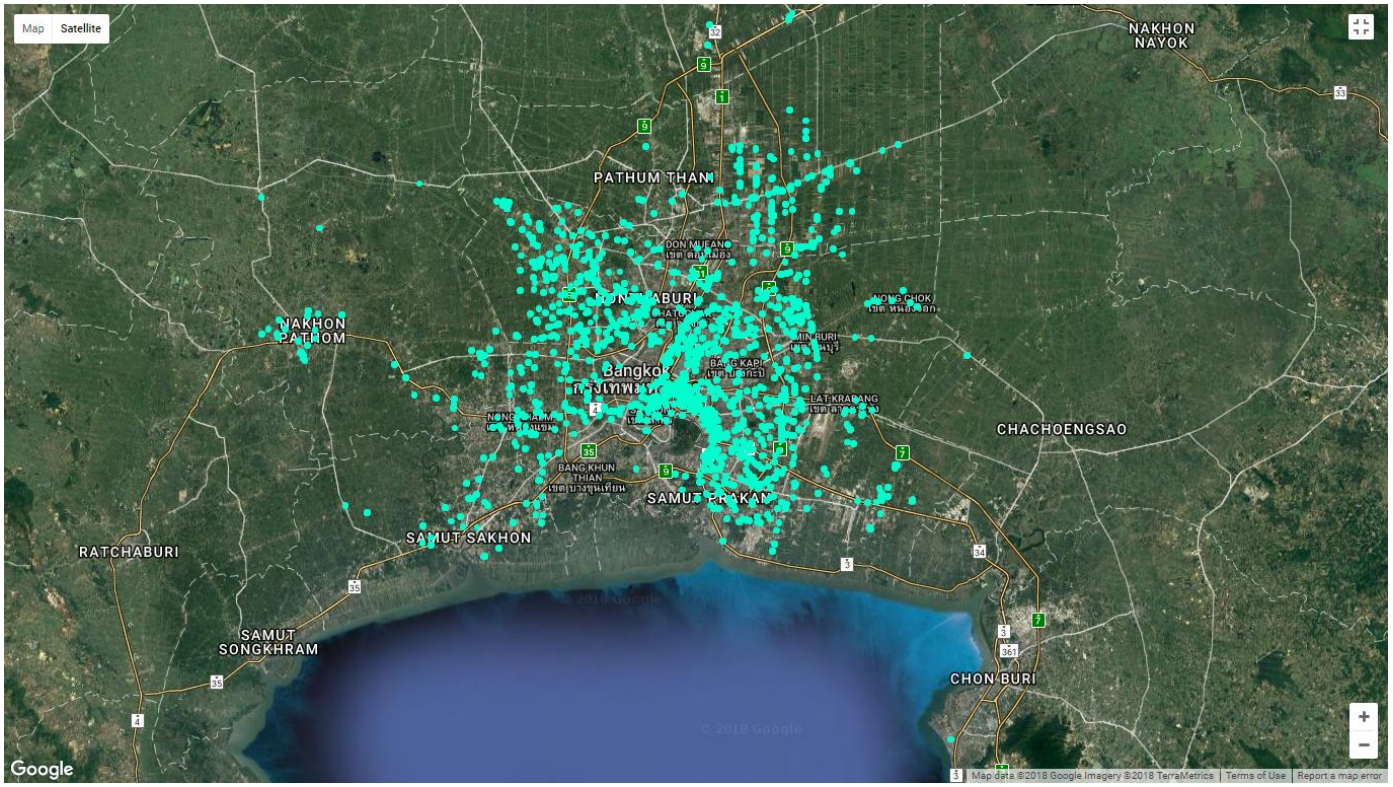


# Example - Real Estate segmentation in Thailand

What should be the input feature of this?



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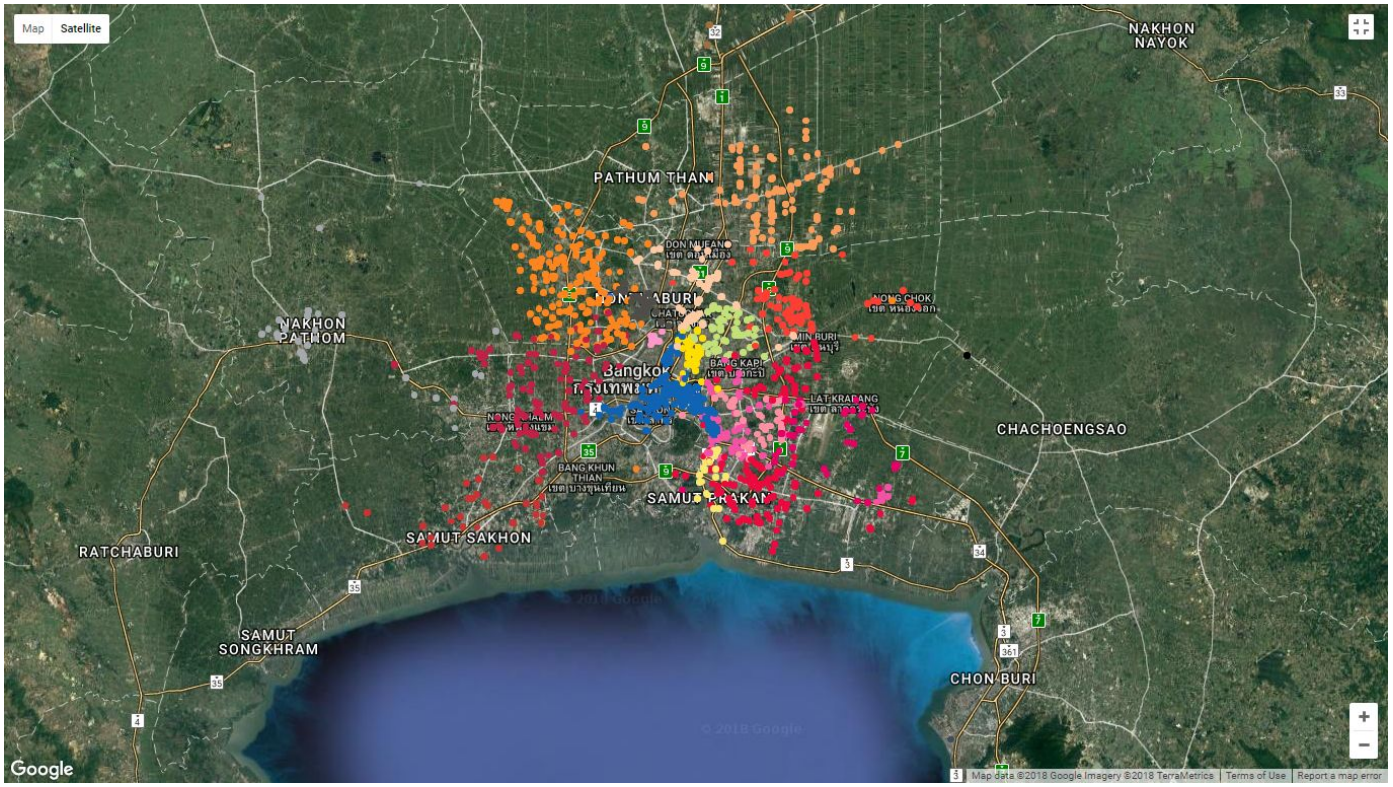

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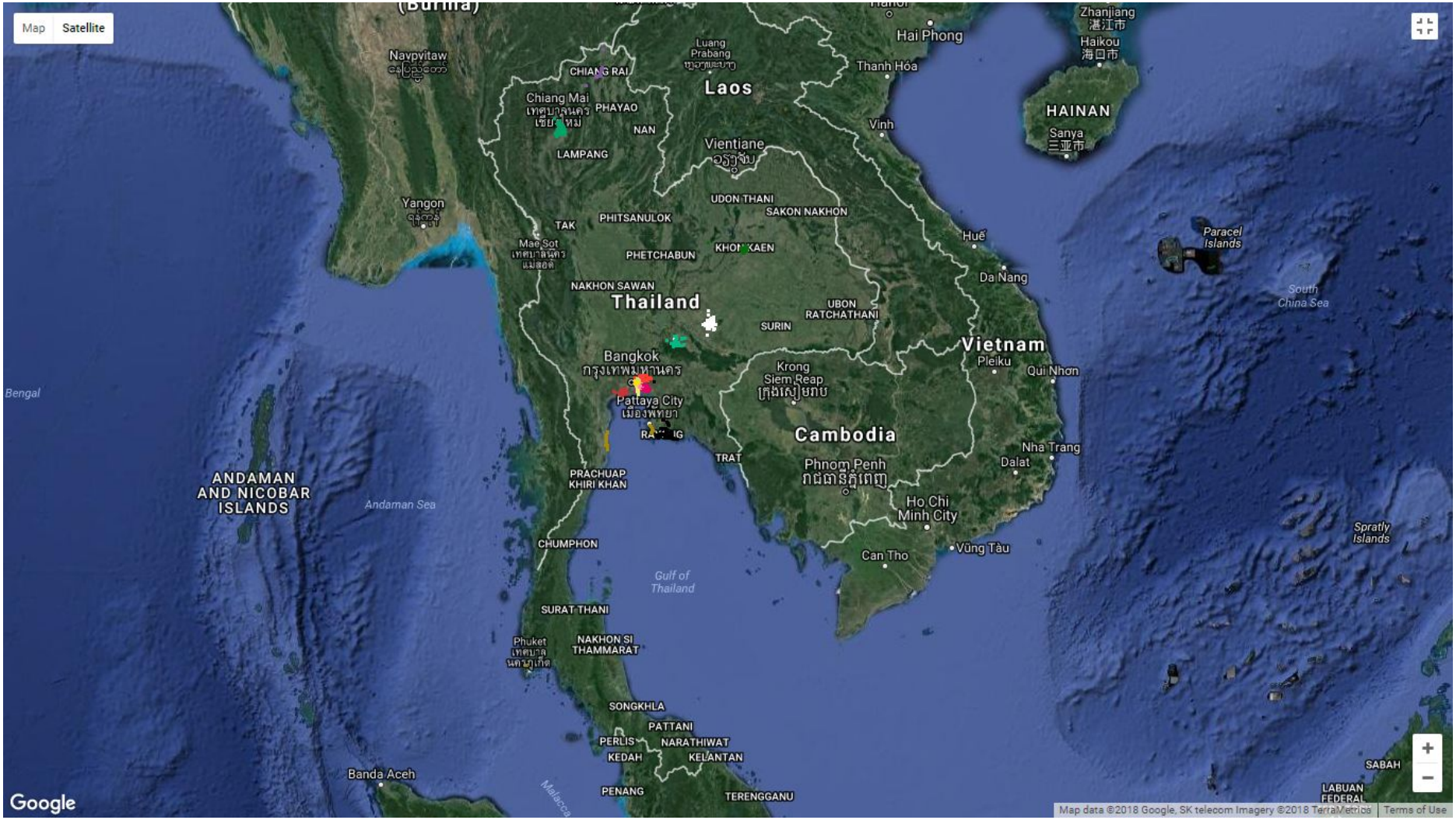

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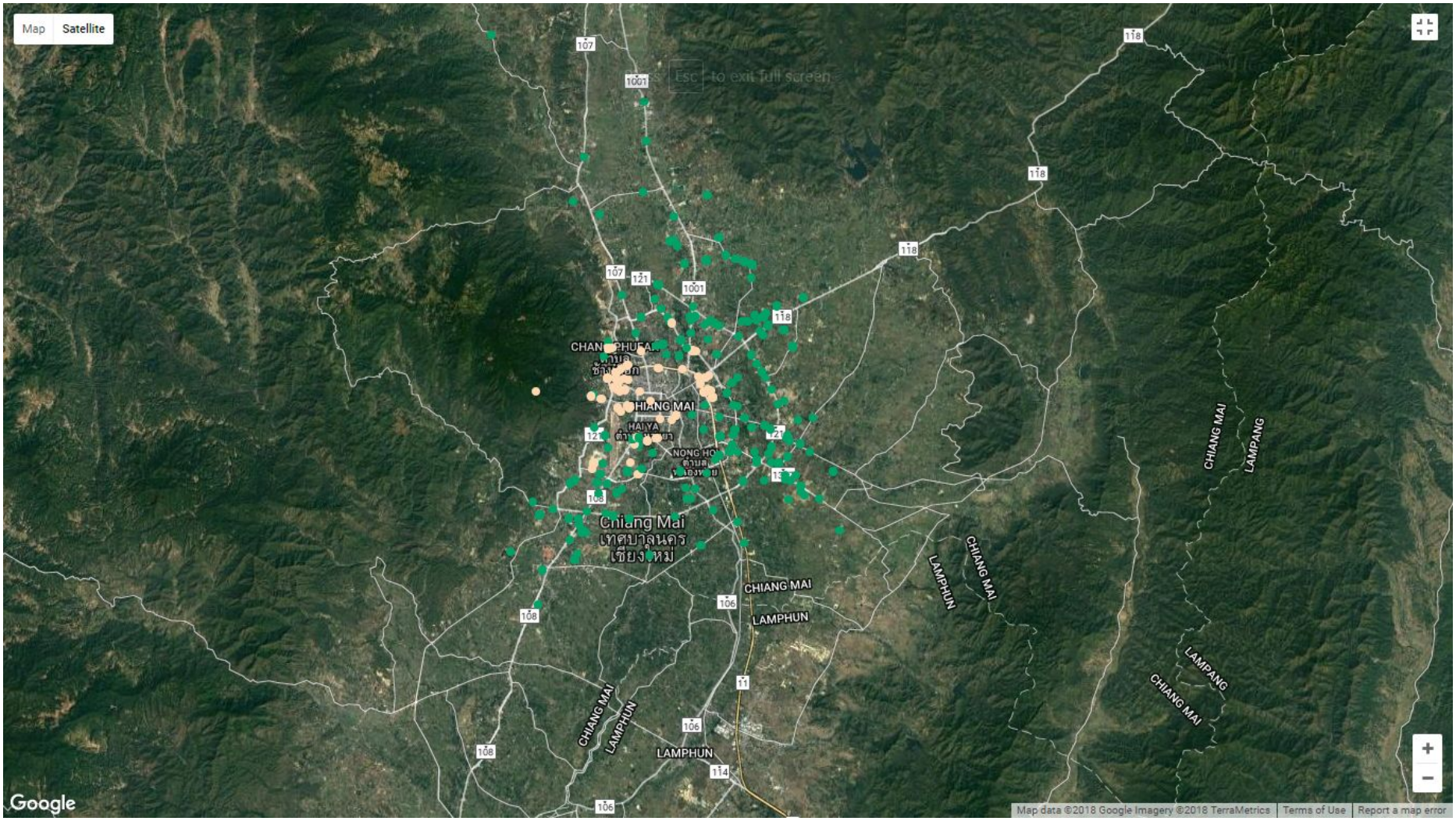

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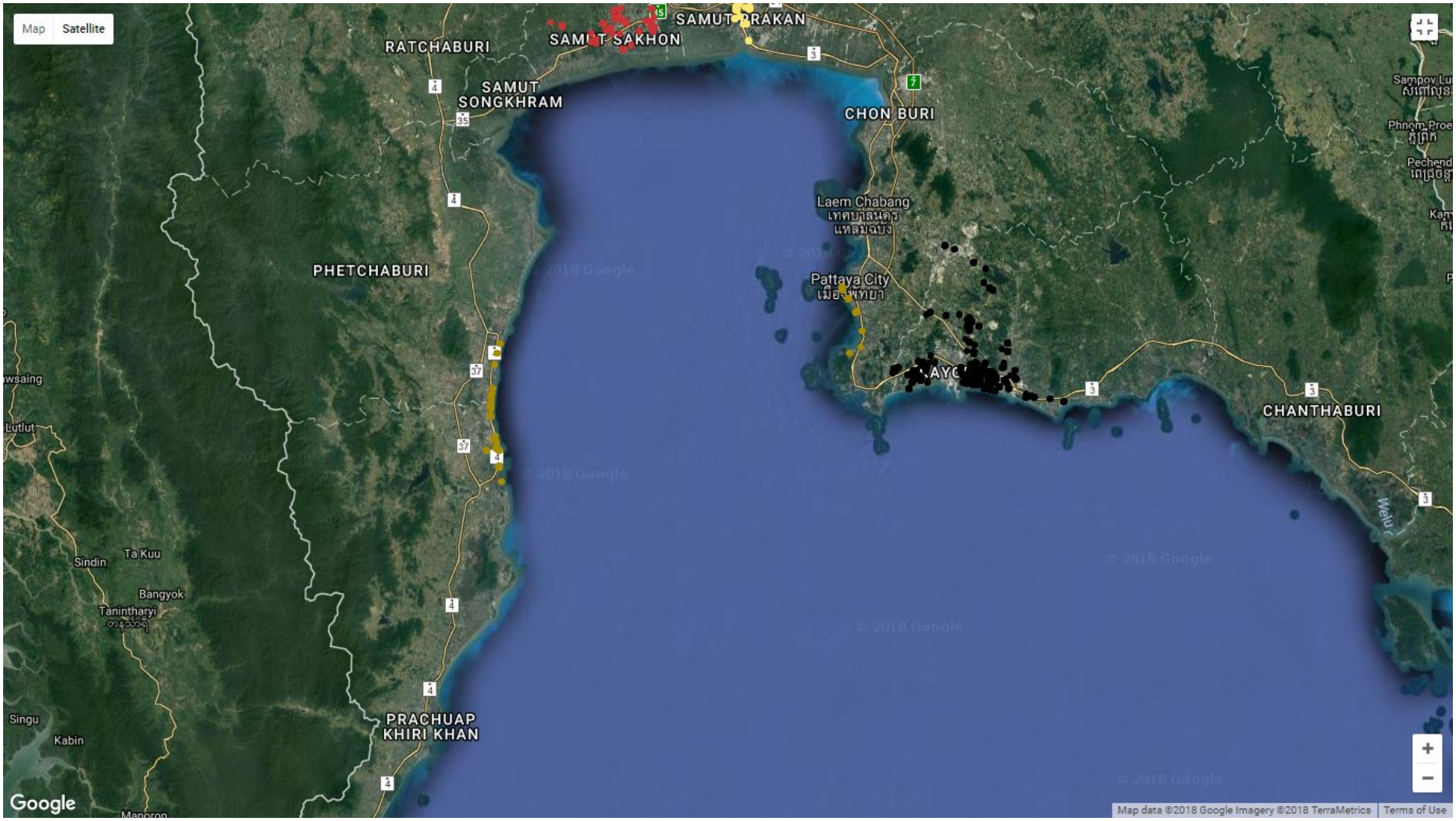

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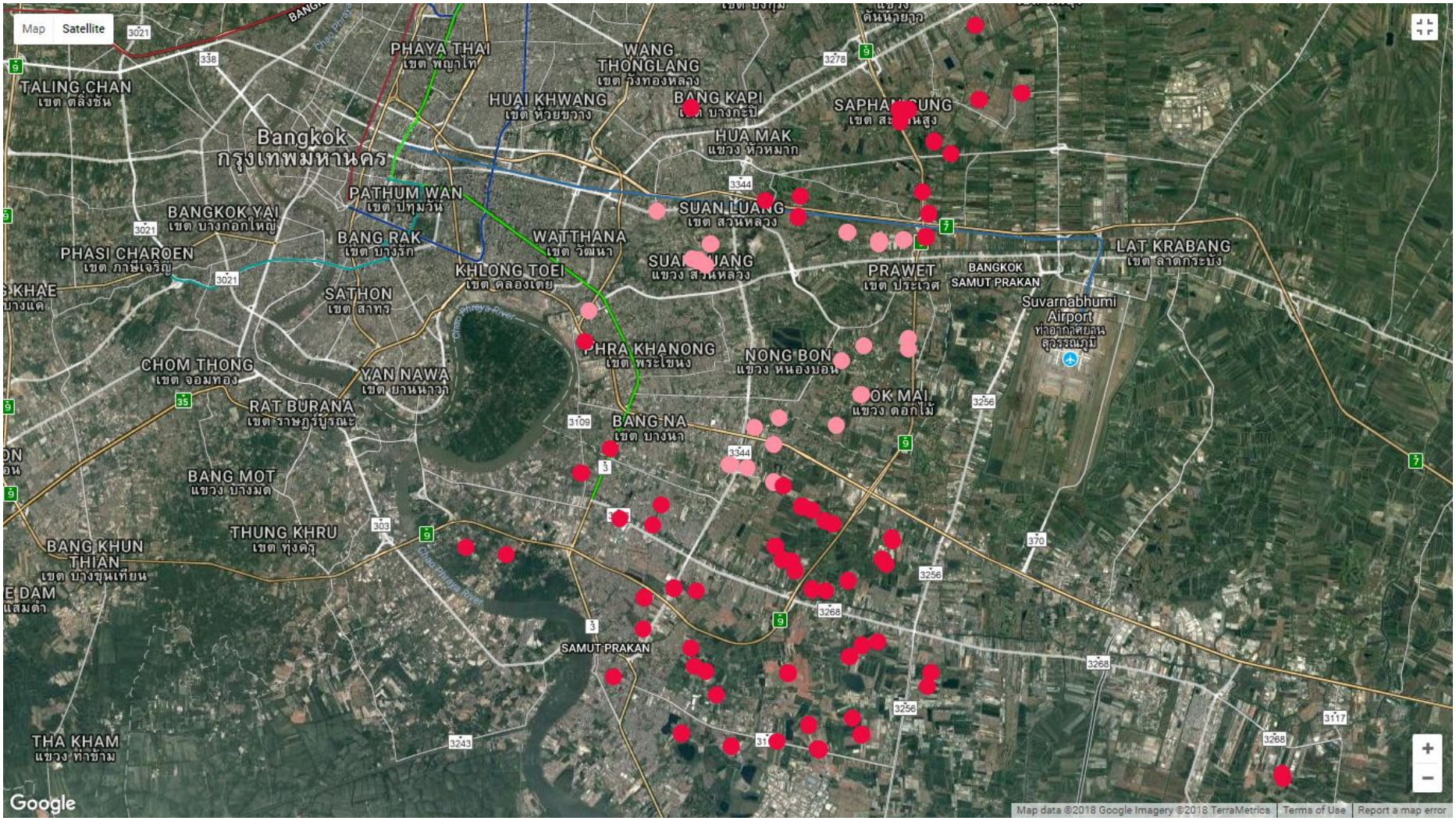
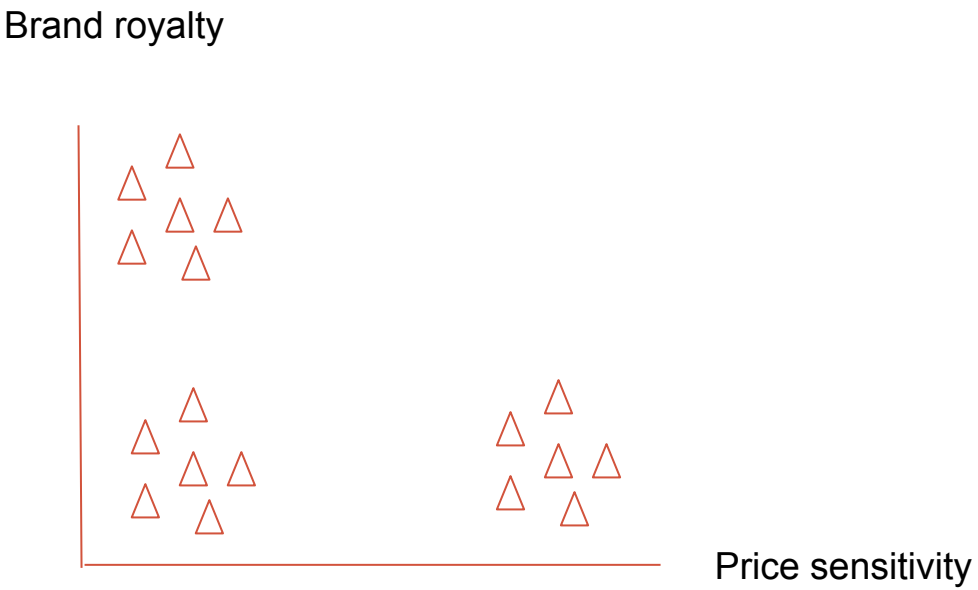


# K-mean clustering

Clustering - task that tries to automatically discover groups within the data

Too hard…



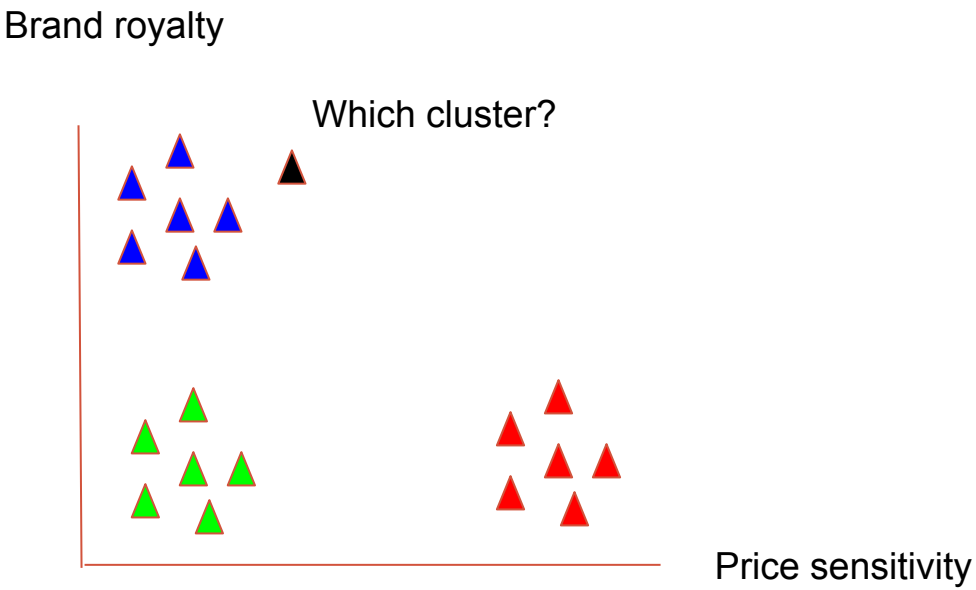
# K-mean clustering

Clustering - task that tries to automatically discover groups within the data

Too hard…

Easier if we know the grouping beforehand (supervised)

How?



# Nearest Neighbour classification

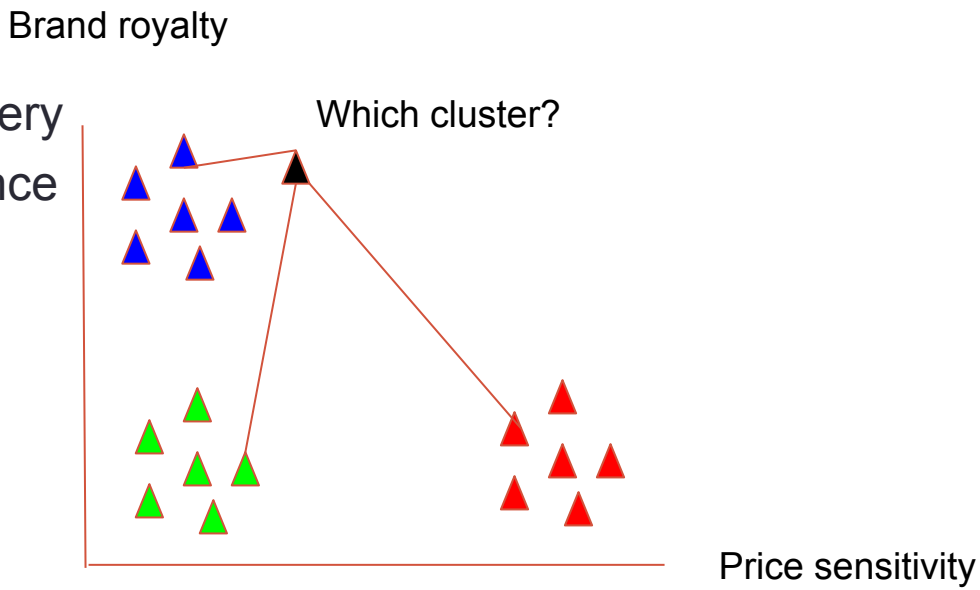
Find the closest training data, assign the same label as the training data

Given query data

For every point in the training data

Compute the distance with the query

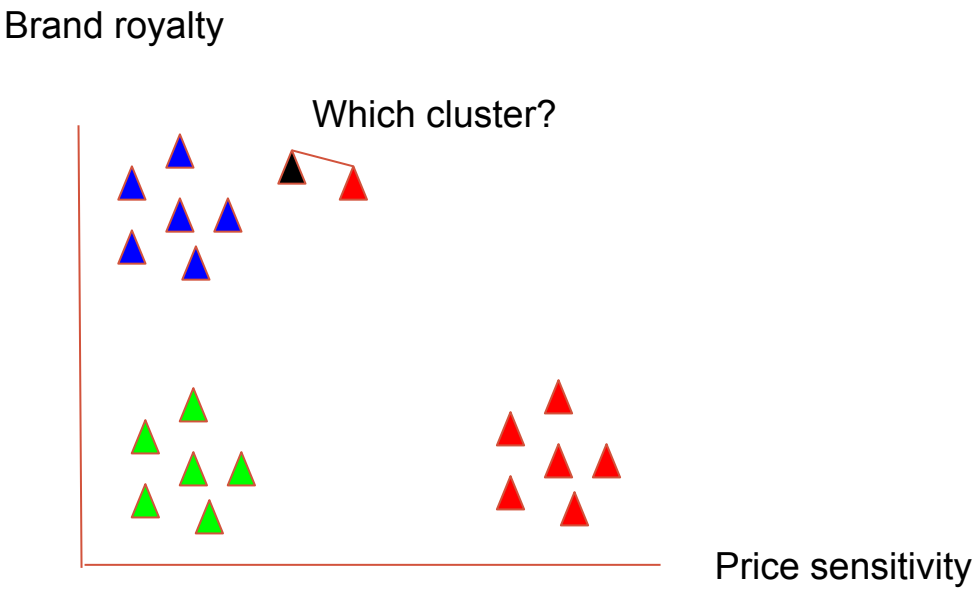
Assign label of the smallest distance



# K-Nearest Neighbour (kNN) classification

Nearest Neighbour is susceptible to noise in the training data

Use a voting scheme instead



# K-Nearest Neighbour (kNN) classification

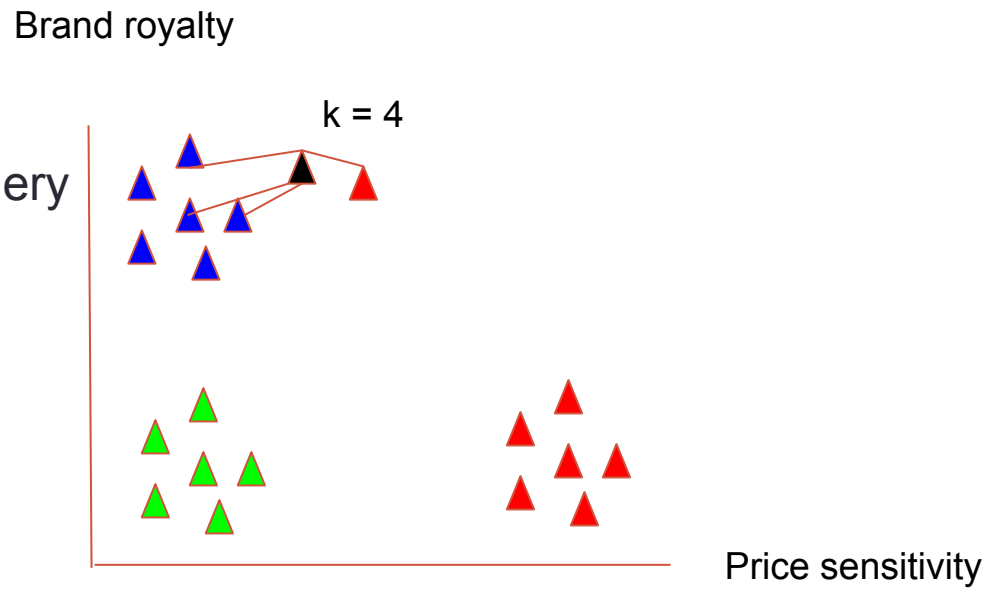
Nearest Neighbour is susceptible to noise in the training data

Use a voting scheme instead

Given query data

For every point in the training data

- Compute the distance with the query
- Find the K closest data points
- Assign label by voting



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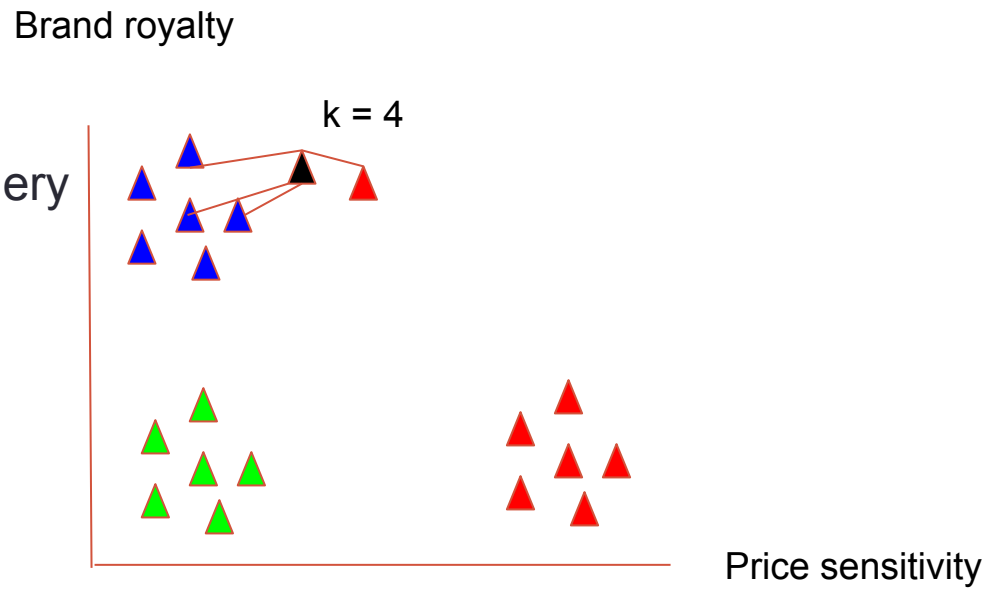



The votes can be weighted by the inverse distance (weighted k-NN)

# Closest?

We need some kind of distance or similarity measures

F($\mathbf{X}_1$ ,$\mathbf{X}_2$) = d

$$X_1 = [x_{1,1}, x_{1,2}, \ldots, x_{1,n}]$$

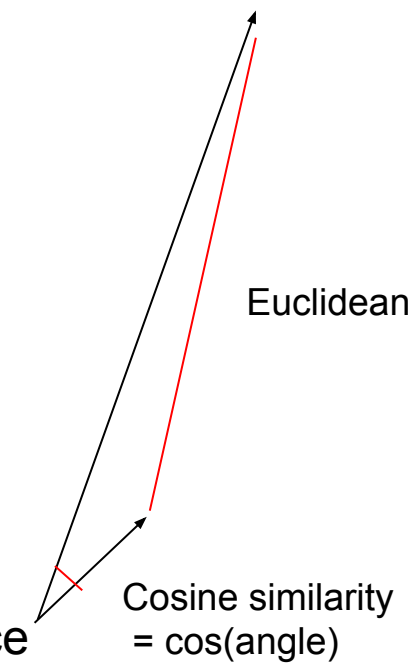
$$X_2 = [x_{2,1}, x_{2,2}, \ldots, x_{2,n}]$$

Euclidean distance

$$\sqrt{\Sigma_i (x_{1,i} - x_{2,i})^2}$$

Cosine similarity

$$\frac{X_1 \cdot X_2}{|X_1||X_2|} = \frac{\Sigma_i x_{1,i} x_{2,i}}{\sqrt{\Sigma_i x_{1,i}^2}\sqrt{\Sigma_i x_{2,i}^2}}$$




Many more distances, Jaccard distance, Earth mover distance

# KNN runtime

For every point in the training data

- Compute the distance with the query
- Find the K closest data points
- Assign label by voting

O(N)

O(JN) - If we have J queries

Expensive

Ways to make it faster

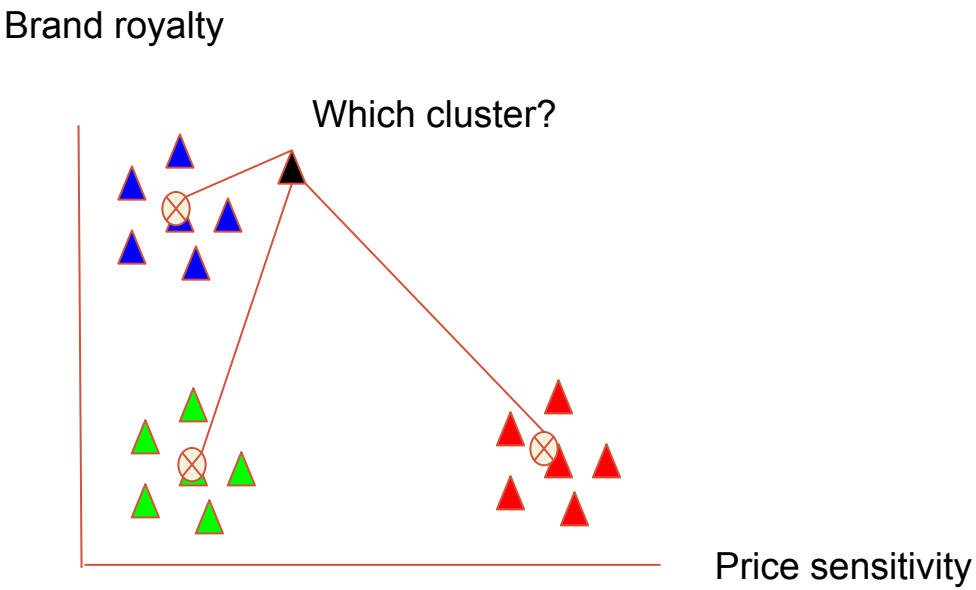
- Kernelized KNN
- Locally Sensitive Hashing (LSH)
- Use centroids

# Centroids

Basically the representative of the cluster

Find the mean location of the cluster by averaging

Can use mode or median depending on the data

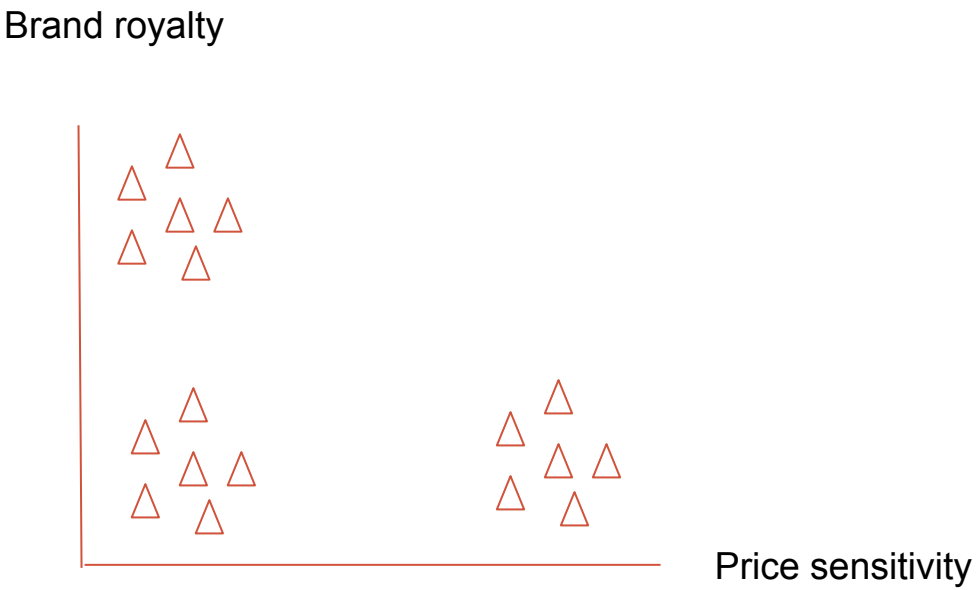



O(JL)

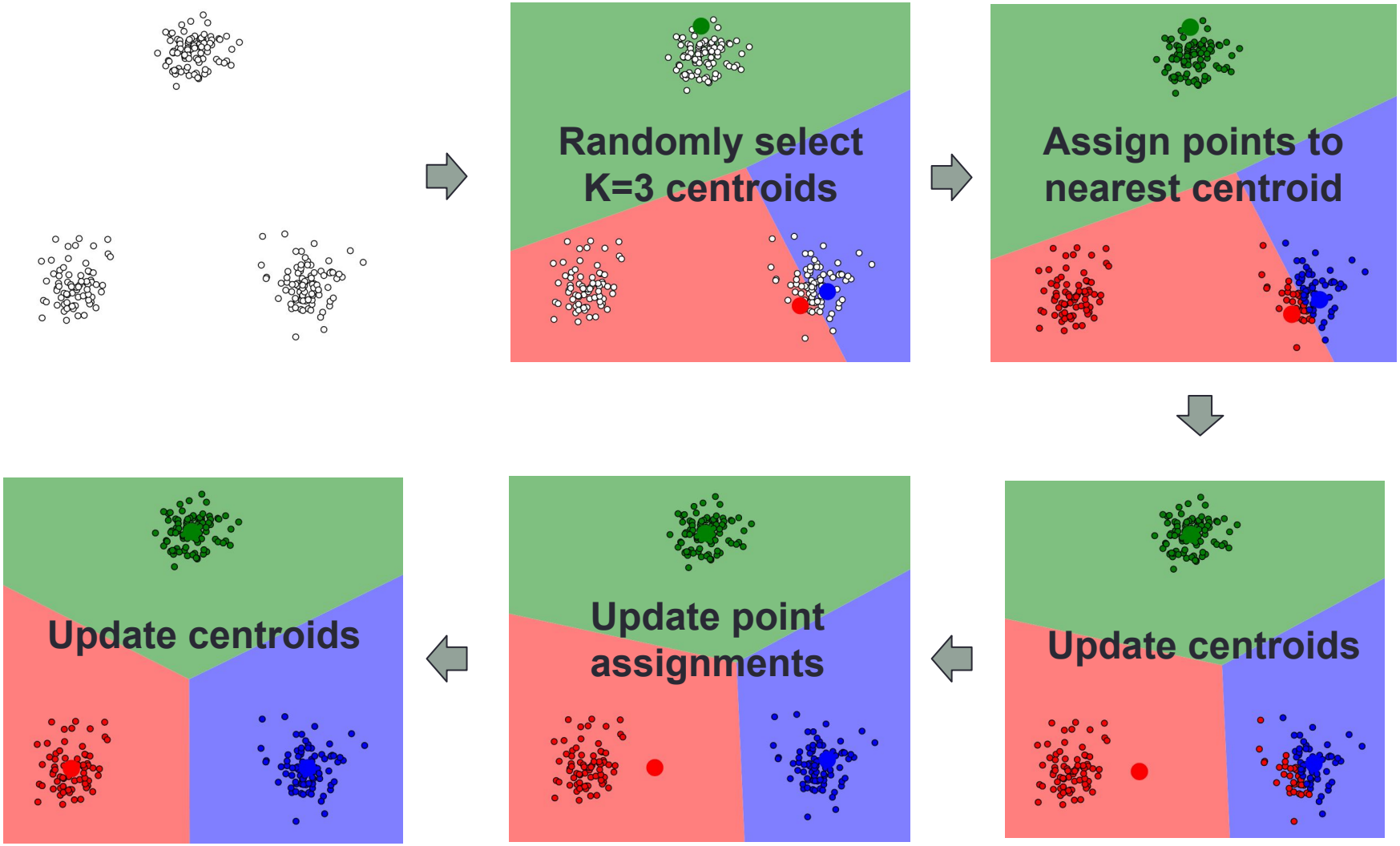
L - number of clusters

# K-mean clustering

1. Randomly k centroids by picking from data points
2. Assign each data points to centroids
3. Update centroids for each cluster
4. Repeat 2-3 until centroids does not change



# An Illustration Of K-Mean Clustering




From https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

# Characteristics of K-means

- **The number of clusters, *K*, is specified in advance.**
- **Always converge to a (local) minimum.**
  - **Poor starting centroid locations can lead to incorrect minima.**

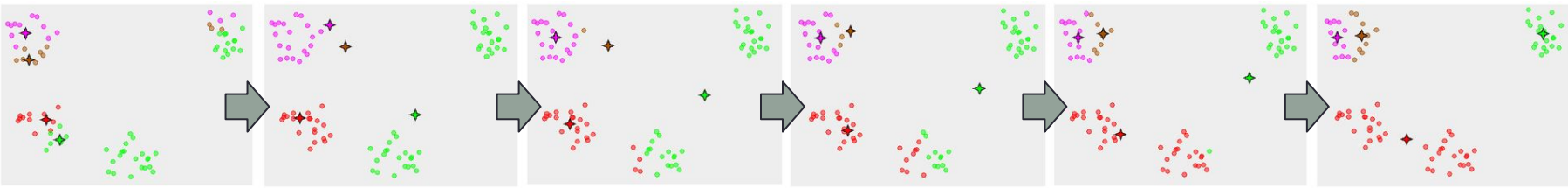
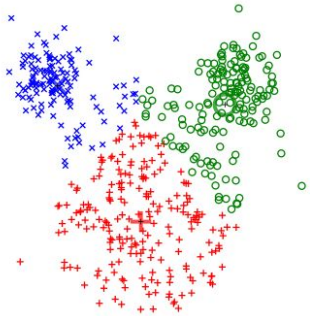
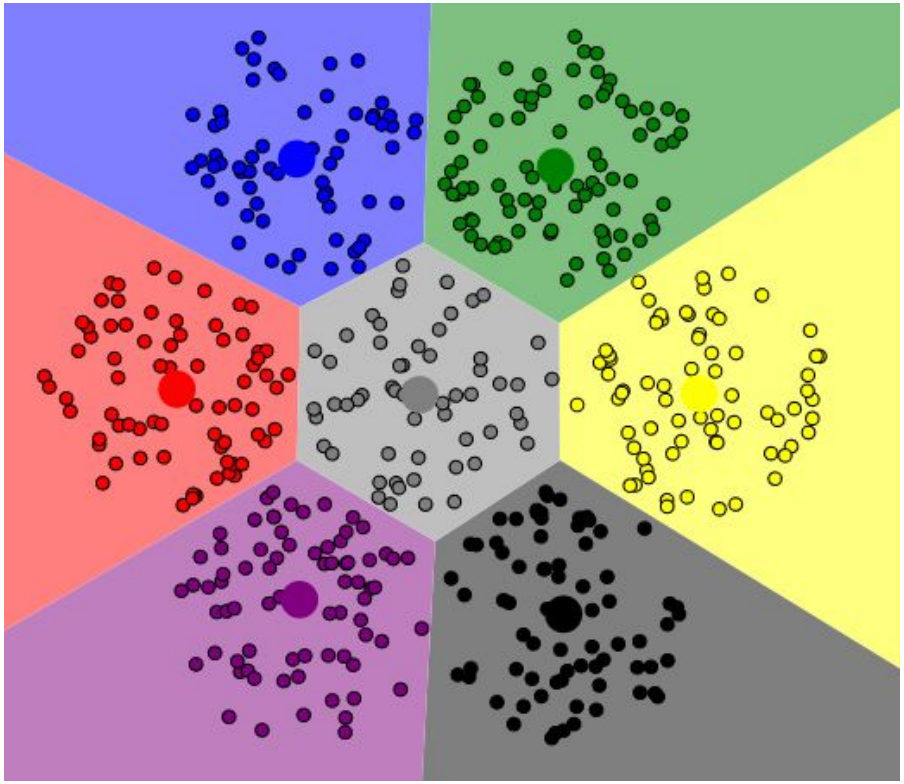


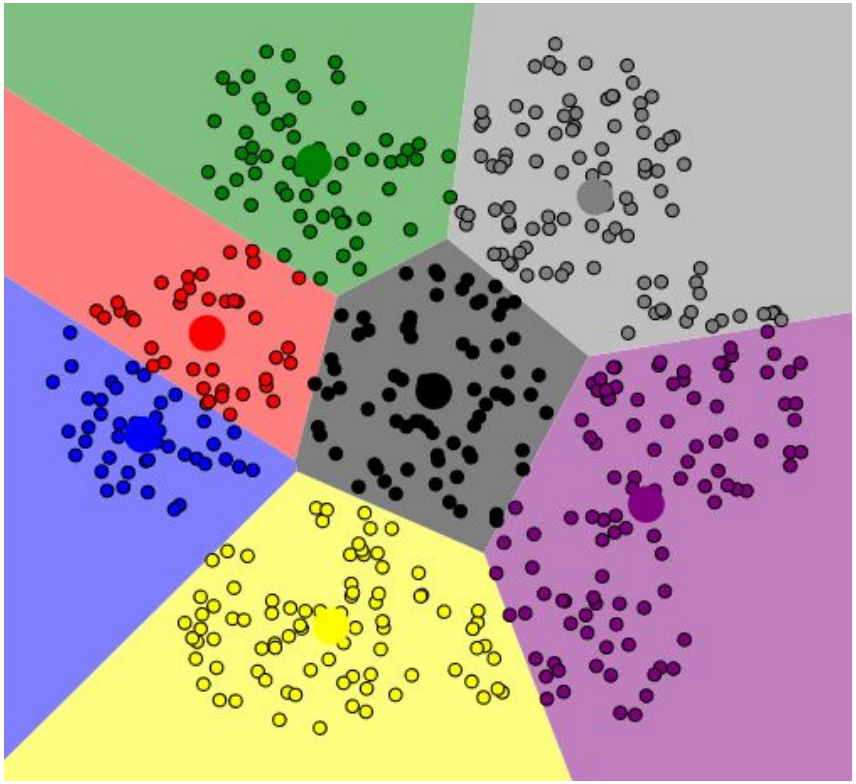
Image from https://en.wikipedia.org/wiki/K-means_clustering

- **The model has several implicit assumptions:**
  - **Data points scatter around cluster's centers.**
  - **Boundary between adjacent clusters is always halfway between the cluster centroids.**



# Effect of bad initializations

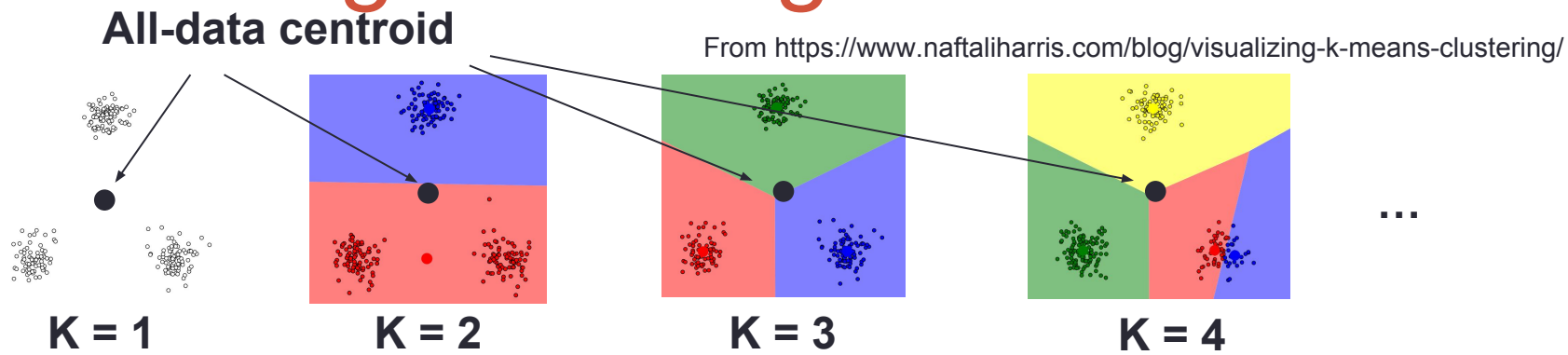




Solution, try different randomization and pick the best

From https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

# Selecting K - Using Elbow method




$$\text{fraction of explained variance} = \frac{\text{between-cluster variance}}{\text{all-data variance}}$$

$$\text{between-cluster variance} = \sum_{i=1}^{K} \frac{n_i (M_i - M)^2}{K-1}$$, where $n_i$ = size of $i^{th}$ cluster,

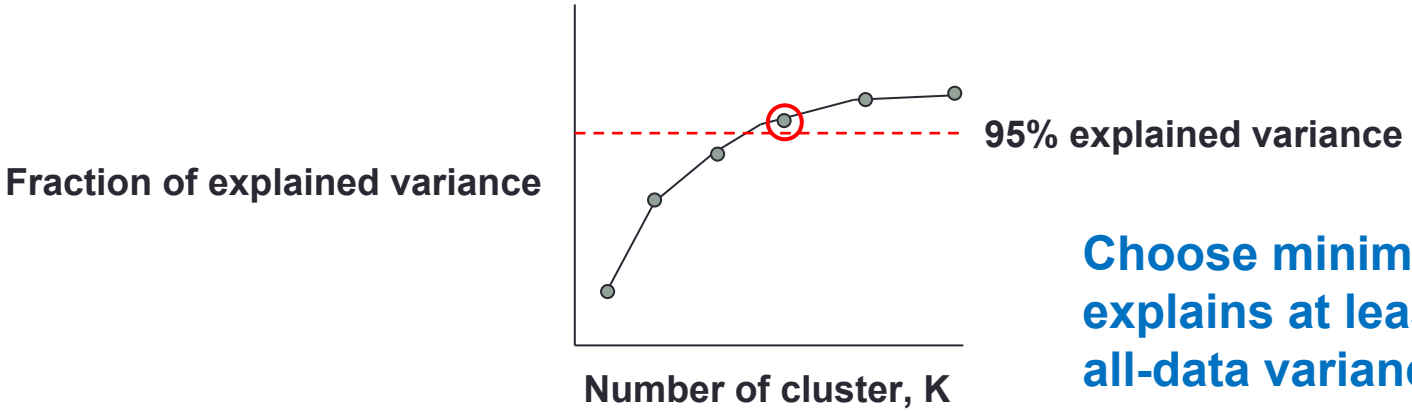
$M_i$ = centroid of $i^{th}$ cluster, and

$M$ = all-data centroid.

$$\text{all-data variance} = \sum_{i=1}^{N} \frac{(x_i - M)^2}{N-1}$$, where $x_i$ = $i^{th}$ data point and N = # of data.

The elbow method chooses K where increasing complexity doesn't yield much in return.

# Selecting K - other methods




**Choose minimal K that explains at least 95% of the all-data variance.**

---

K = 2

K = 3

K = 4

⋮

→ **Training K-mean Clustering Model** → **Testing / Cross-validation** →

| K | Accuracy |
|---|---|
| 2 | 50% |
| 3 | 68% |
| 4 | 83% |
| ⋮ | ⋮ |

**Choose K that maximizes certain objective (e.g. accuracy on testing data)**

Best method

# REGRESSION

with some K-mean clustering

# Let’s look at another example

https://soclaimon.wordpress.com/2015/07/24/%E0%B9%82%E0%B8%A1%E0%B9%80%E0%B8%94%E0%B8%A5%E0%B8%99%E0%B9%89%E0%B8%B33%E0%B8%A2%E0%B8%B8%E0%B8%84%E0%B8%A1%E0%B8%B2%E0%B8%A3%E0%B9%8C%E0%B8%84-%E0%B8%9B%E0%B8%B9/

# Predicting amount of rainfall

https://esan108.com/%E0%B8%9E%E0%B8%A3%E0%B8%B0%E0%B9%82%E0%B8%84%E0%B8%81%E0%B8%B4%E0%B8%99%E0%B8%AD%E0%B8%B0%E0%B9%84%E0%B8%A3-%E0%B8%AB%E0%B8%A1%E0%B8%B2%E0%B8%A2%E0%B8%96%E0%B8%B6%E0%B8%87.html

# Predicting amount of rainfall

| Cloth | Corn | Grass | Water | Beer | Rainfall |
|---|---|---|---|---|---|
| 4 | 6 | 3 | 10 | 0 | **76950** |
| 5 | 1 | 0 | 0 | 7 | **30234** |
| 6 | 0 | 3 | 5 | 7 | **123456** |
| 5 | 0 | 3 | 12 | 0 | **89301** |
| 4 | 3 | 0 | 6 | 7 | **?** |

We assume the input features have some correlation with the amount of rainfall.

Can we create a model that predict the amount of rainfall?

What is the output?

What is the input (features)?

# Predicting the amount of rainfall

- The correlation can be positive or negative

# Predicting the amount of rainfall

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| 4 | 3 | 0 | 6 | 7 | **?** |

- $h_{\boldsymbol{\theta}}(\mathbf{x_1}) = \theta_0 + \theta_1 x_{1,1} + \theta_2 x_{1,2} + \theta_3 x_{1,3} + \theta_4 x_{1,4} + \theta_5 x_{1,5}$

  1 refers to index of the data (the first in the training/test set)
- Where θs are the parameter of the model
- Xs are values in the table

# (Linear) Regression

- $h_{\boldsymbol{\theta}}(\mathbf{x_1}) = \theta_0 + \theta_1 x_{1,1} + \theta_2 x_{1,2} + \theta_3 x_{1,3} + \theta_4 x_{1,4} + \theta_5 x_{1,5}$
- θs are the parameter (or weights)

Assume $x_0$ is always 0

- We can rewrite

n is dimension of x

$$h_\theta(\mathbf{x}_i) = \Sigma_{j=0}^{n} \theta_j x_{i,j} = \theta^T \mathbf{x}_i$$

h is parameterized by θ

- Notation: vectors are bolded
- Notation: vectors are column vectors

# Picking $\boldsymbol{\theta}$

- Random until you get the best performance?

- How to quantify best performance?

$$h_\theta(\mathbf{x}_i) = \Sigma_{j=0}^{n} \theta_j x_{i,j} = \theta^T \mathbf{x}_i$$

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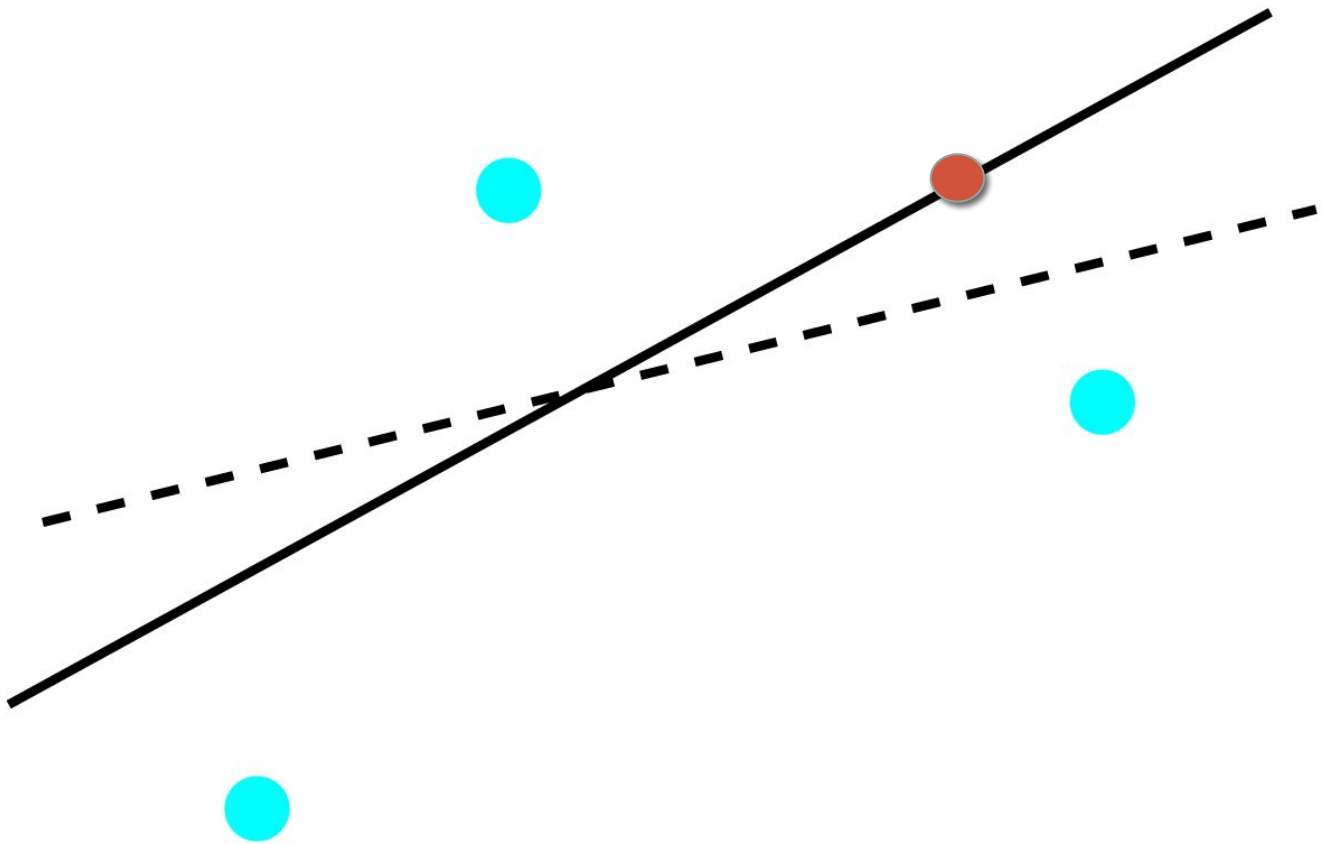

https://chem.libretexts.org/Textbook_Maps/Analytical_Chemistry_Textbook_Maps/Map%3A_Analytical_Chemistry_2.0_(Harvey)/05_Standardizing_Analytical_Methods/5.4%3A_Linear_Regression_and_Calibration_Curves

# Cost function (Loss function)

- Let's use the mean square error (MSE)

m is the number of training examples

$$J(\theta) = \frac{1}{m}\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x_i})^2$$

i here is the index of the training example
Note how **x** is bolded

We want to pick **θ** that minimize the loss

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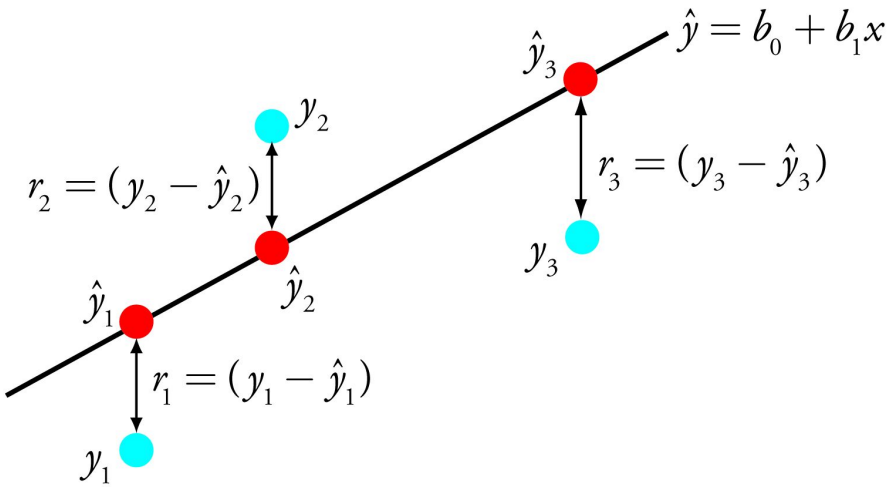

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$$\frac{m}{2}J(\theta) = \boxed{\frac{1}{2}\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x_i})^2}$$

# Picking $\boldsymbol{\theta}$

- Random until you get the best performance?
  - Can we do better than random chance?

- How to quantify best performance?

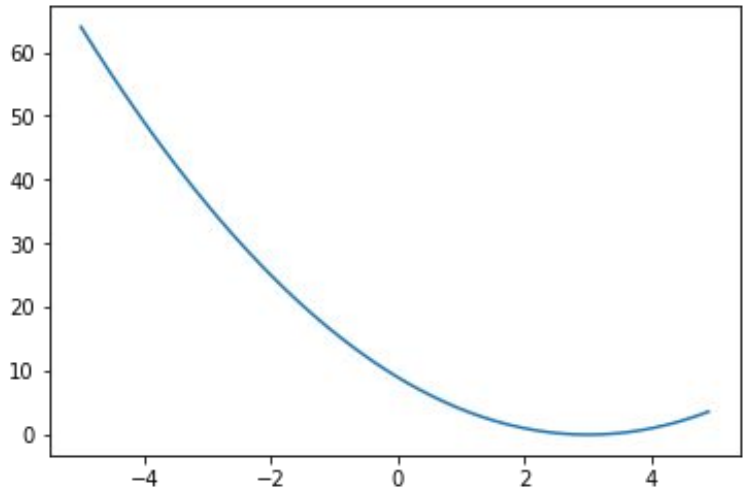
$$\frac{m}{2}J(\theta) = \frac{1}{2}\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x_i})^2$$

# Minimizing a function

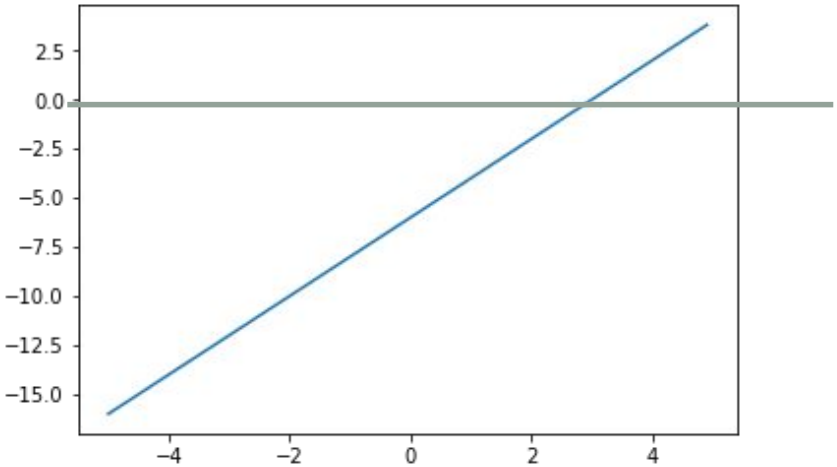
- You have a function
  - $y = (x - a)^2$
- You want to minimize Y with respect to x
  - $dy/dx = 2x - 2a$
  - Take the derivative and set the derivative to 0
    - (And maybe check if it's a minima, maxima or saddle point)

- We can also go with an iterative approach

# Gradient descent



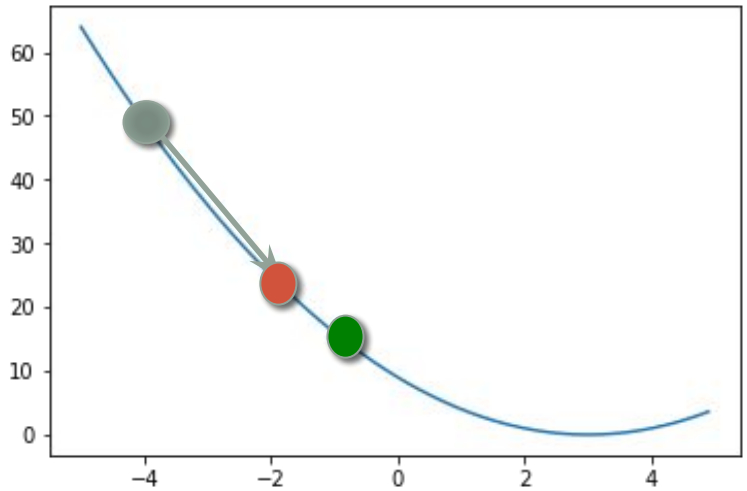

y




dy/dx

First what does dy/dx means?

# Gradient descent

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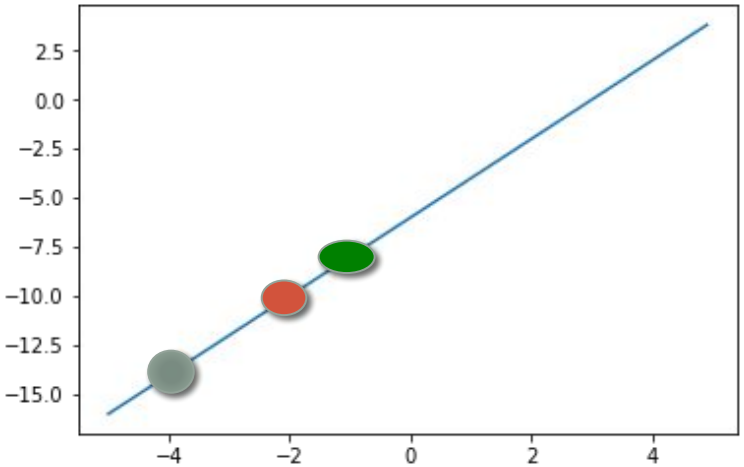
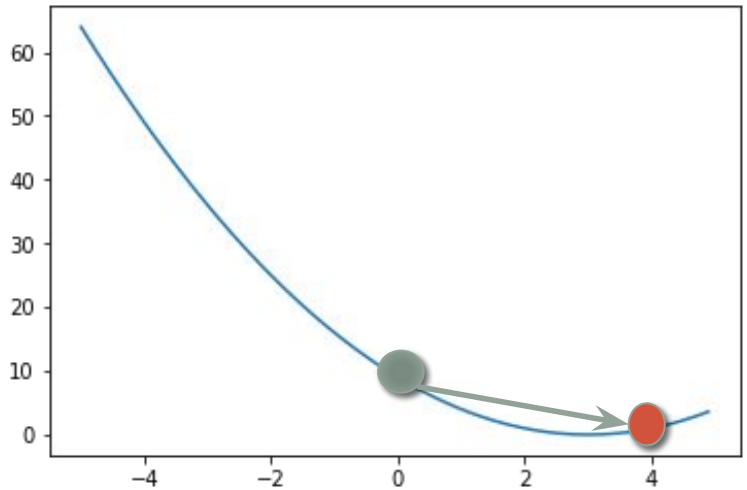


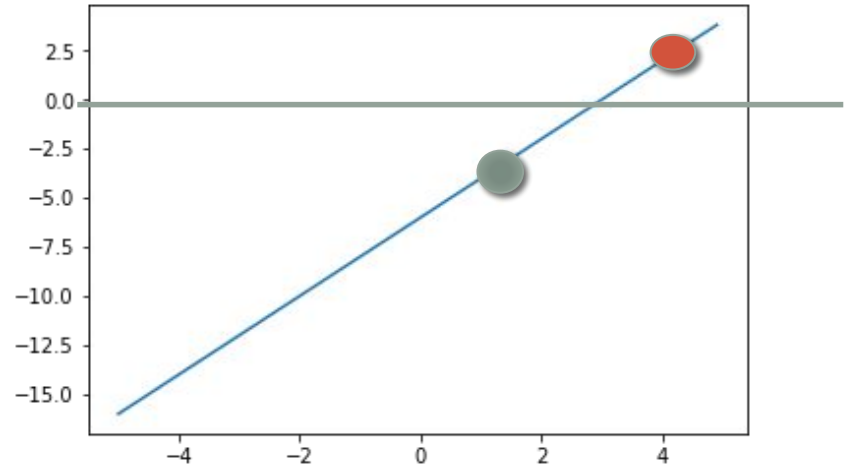

dy/dx

Move along the negative direction of the gradient
The bigger the gradient the bigger step you move

# Gradient descent



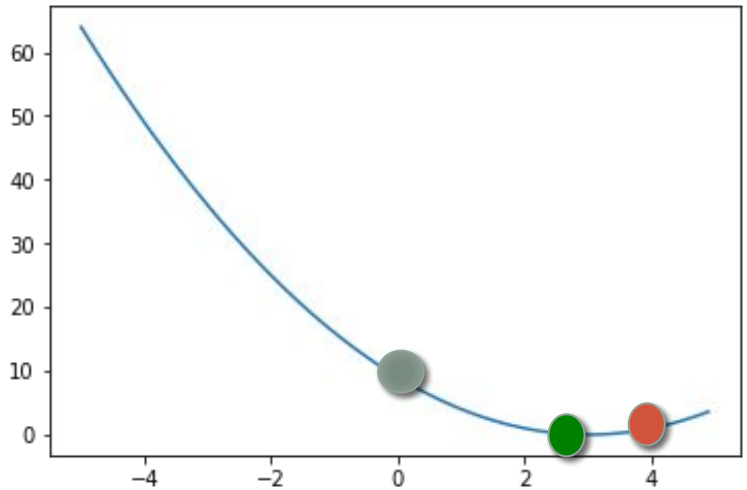

y



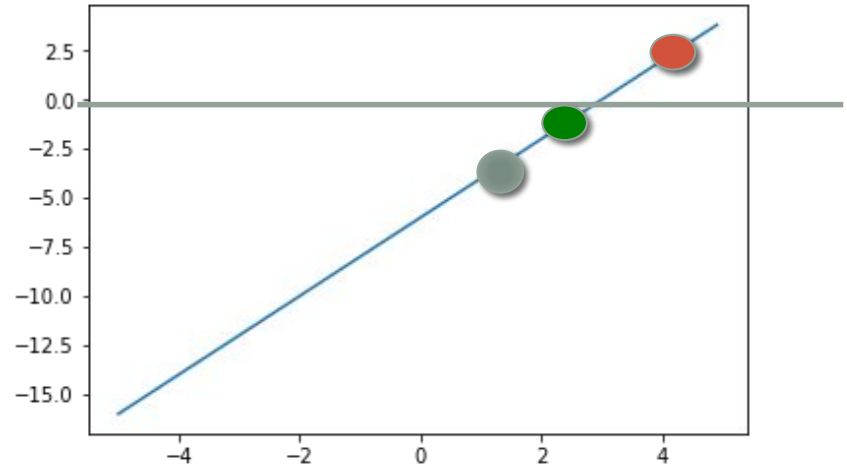

dy/dx

What happens when you overstep?

# Gradient descent



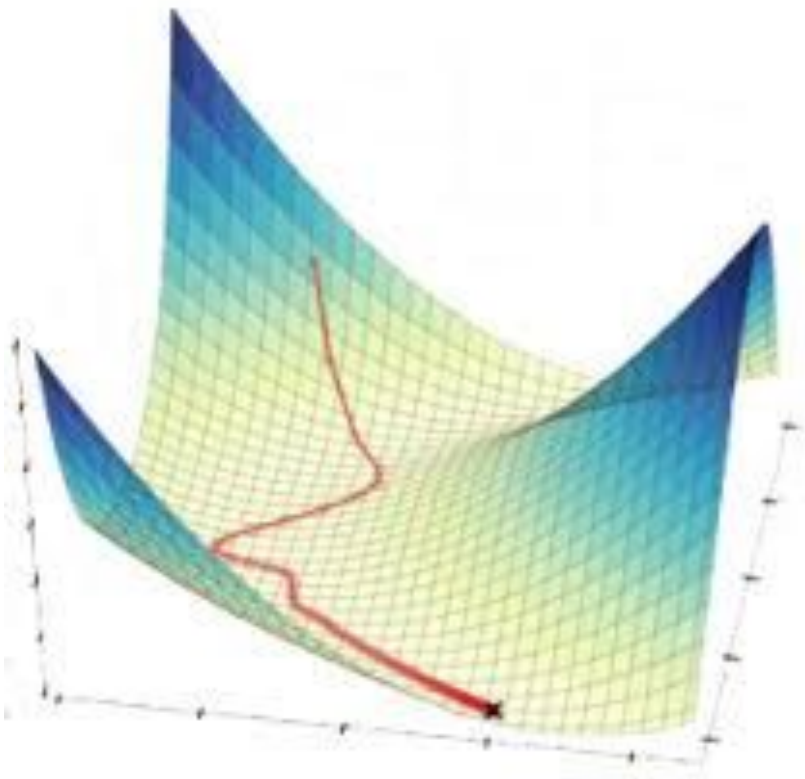

y




dy/dx

If you over step you can move back

# Gradient descent in 3d



http://dsdeepdive.blogspot.com/2016/03/optimizations-of-gradient-descent.html

# Formal definition

- $y = f(x)$

- Pick a starting point $x_0$

- Moves along -dy/dx
- $x_{n+1} = x_n - r * dy/dx$
- Repeat till convergence
- r is the learning rate

  Big r means you might overstep

  Small r and you need to take more steps

# Picking $\boldsymbol{\theta}$

- Random until you get the best performance?
  - Can we do better than random chance?
    - Gradient descent (a better guess!)

- How to quantify best performance?

$$\frac{m}{2}J(\theta) = \frac{1}{2}\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x_i})^2$$

# LMS regression with gradient descent

$$J(\theta) = \frac{1}{2}\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x_i})^2$$

$$\frac{\partial J}{\partial \theta_j} = -\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

# LMS regression with gradient descent

$$\frac{\partial J}{\partial \theta_j} = -\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

Interpretation?

# Batch updates vs mini-batch

$$\theta_j \Leftarrow \theta_j - r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

- Batch updates (considering the whole training data) estimate the Loss function precisely
  - Can takes a long time if m is large
- Updates with a subset of m
  - We now have an estimate of the loss function
    - This can lead to a wrong direction, but we get faster updates
  - Called Stochastic Gradient Descent (SGD) or incremental gradient descent

# Other loss functions

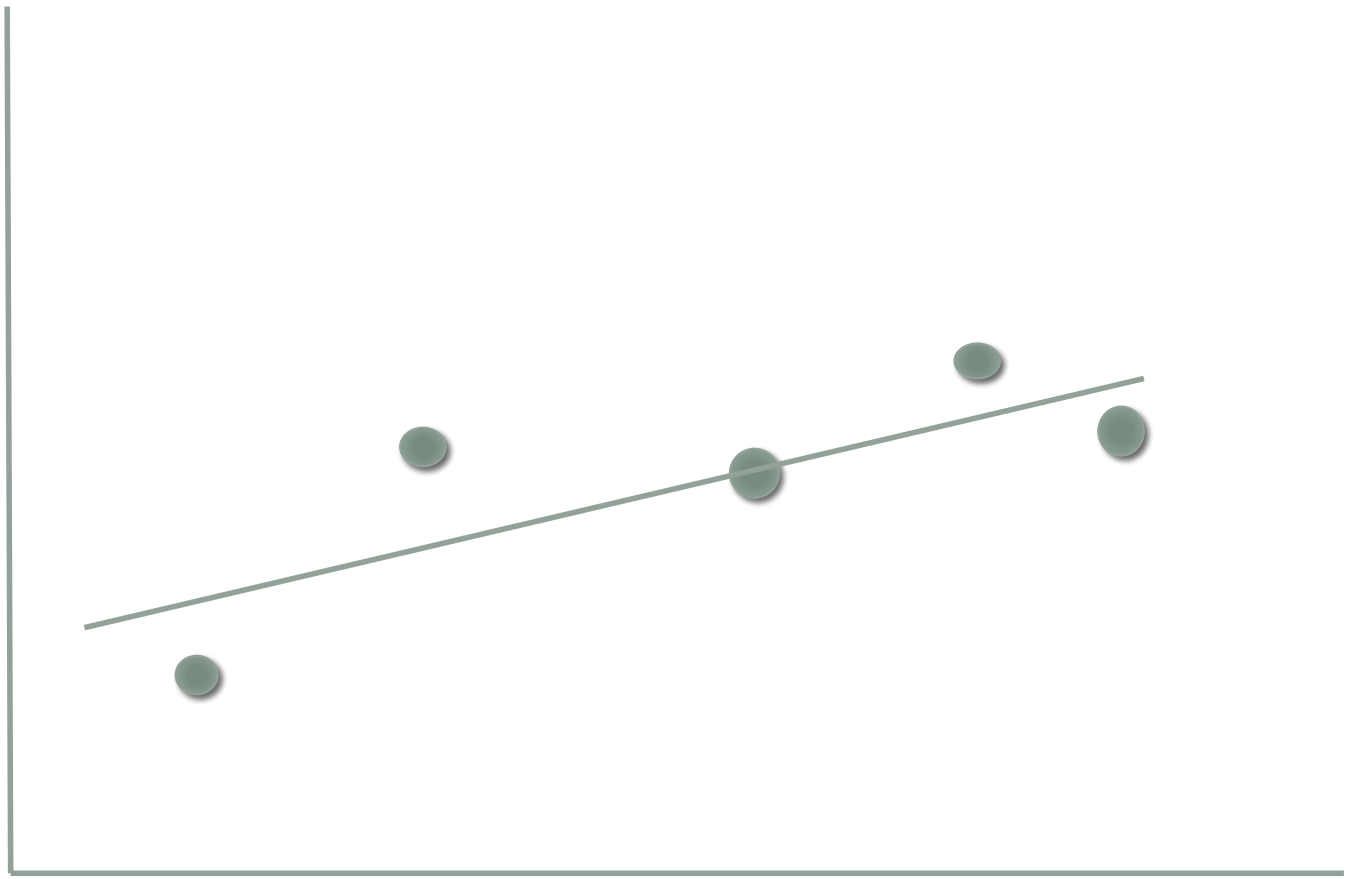
- MSE

$$J(\theta) = \frac{1}{m}\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x_i})^2$$

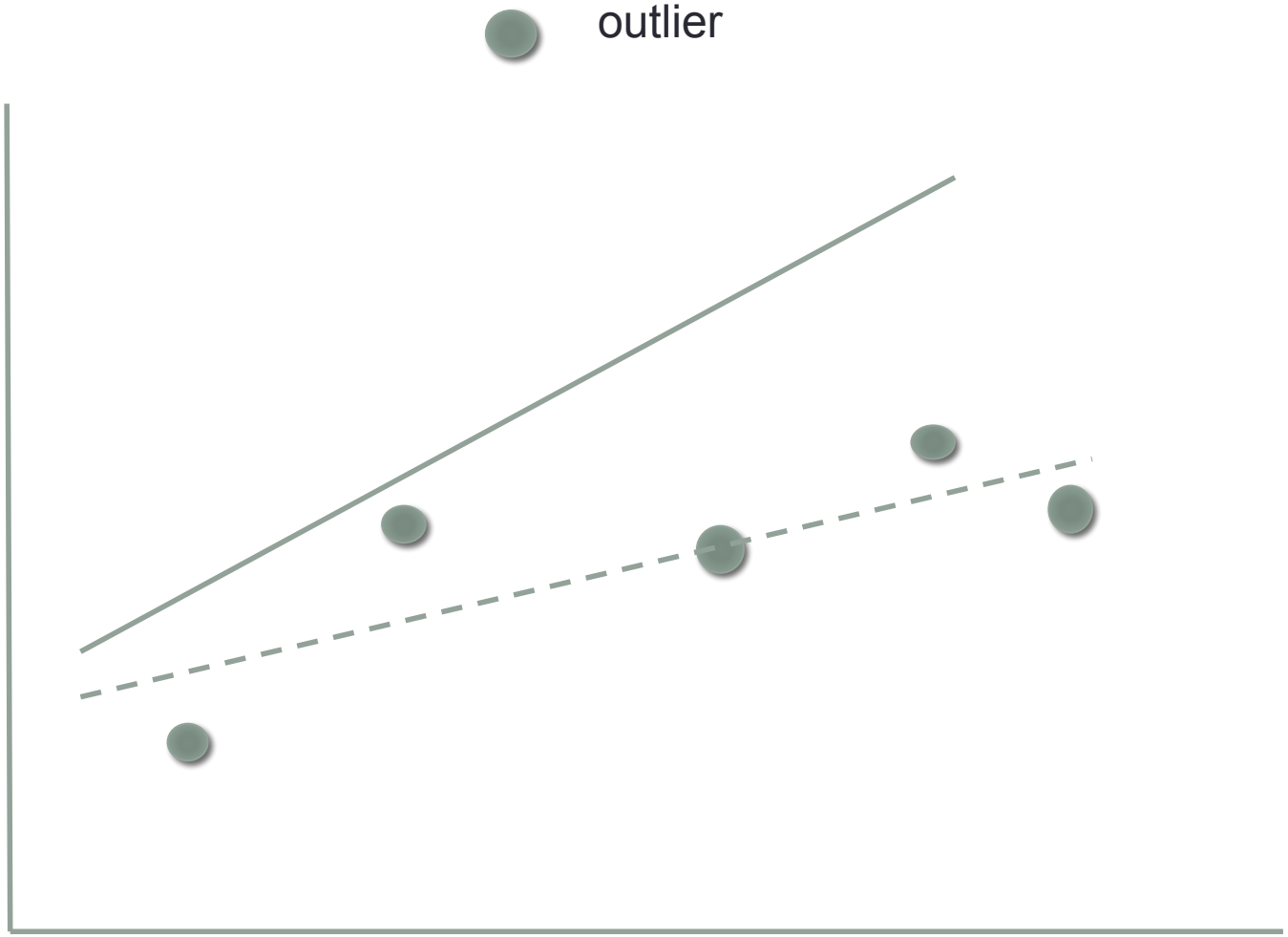
  - Also called L2 loss
- L1 loss

$$\frac{1}{m}\Sigma_{i=1}^{m}|y_i - \theta^T \mathbf{x_i}|$$

# L2 vs L1 loss



# L2 vs L1 loss




Outlier frequently happens in the real world

# Norms (p-norm or Lp-norm)

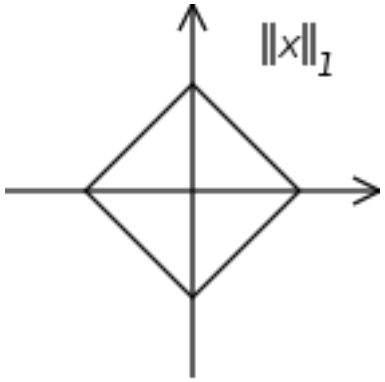
- For any real number p > 1

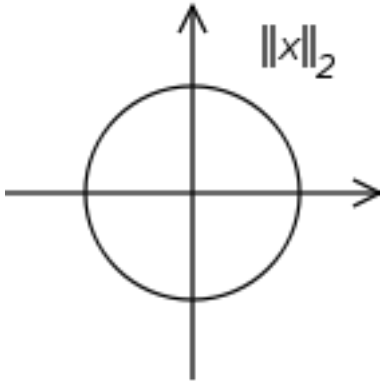
$$||\mathbf{x}||_p = (|x_1|^p + |x_2|^p + ... + |x_n|^p)^{\frac{1}{p}}$$

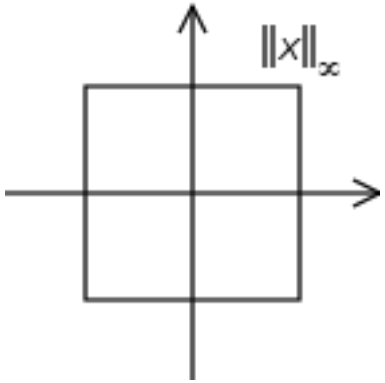
- For p = ∞

$$\|x\|_\infty = \max\{|x_1|, |x_2|, \ldots, |x_n|\}$$

- We'll see more of p-norms when we get to neural networks




https://en.wikipedia.org/wiki/Lp_space

# Minimizing a function

- You have a function
  - $y = (x - a)^2$
- You want to minimize Y with respect to x
  - $dy/dx = 2x - 2a$
  - Take the derivative and set the derivative to 0
    - (And maybe check if it's a minima, maxima or saddle point)

- We can also go with an iterative approach (Gradient descent)

# LMS regression with matrix derivatives

- First let's definite what's a derivative of a matrix
- For a function $f : \mathbb{R}^{m \times n} \mapsto \mathbb{R}$
- The derivative wrt to A is

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial f}{\partial A_{11}} & \cdots & \frac{\partial f}{\partial A_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial A_{m1}} & \cdots & \frac{\partial f}{\partial A_{mn}} \end{bmatrix}$$

http://cs229.stanford.edu/notes/cs229-notes1.pdf

# Example

- Suppose

$$f : \mathbb{R}^{m \times n} \mapsto \mathbb{R}$$

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \qquad \nabla_A f(A) = \begin{bmatrix} \frac{\partial f}{\partial A_{11}} & \cdots & \frac{\partial f}{\partial A_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial A_{m1}} & \cdots & \frac{\partial f}{\partial A_{mn}} \end{bmatrix}$$

$$f(A) = \frac{3}{2} A_{11} + 5 A_{12}^2 + A_{21} A_{22}$$

$$\nabla_A f(A) = \begin{bmatrix} \frac{3}{2} & 10 A_{12} \\ A_{22} & A_{21} \end{bmatrix}$$

# Trace of a matrix

- trA is the sum of the diagonals of matrix A (A must be a square matrix)

$$trA = \Sigma_i^N A_{ii}$$

- Trace of a real number? (1x1 matrix)

# Trace properties

- tr (a) = a
- trA = trA$^T$
- tr(A+B) = trA+trB
- tr(aA) = atr(A)

$$\nabla_A trAB = B^T$$
$$\nabla_{A^T} f(A) = (\nabla_A f(A))^T$$
$$\nabla_A trABA^TC = CAB + C^TAB^T$$
$$\nabla_{A^T} trABA^TC = B^TA^TC^T + BA^TC$$

# LMS regression with matrix derivatives

$$X = \begin{bmatrix} - & x_1^T & - \\ - & x_2^T & - \\ - & x_m^T & - \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ y_m \end{bmatrix}$$

$$X\theta - y = \begin{bmatrix} x_1^T\theta \\ | \\ x_m^T\theta \end{bmatrix} - \begin{bmatrix} y_1 \\ | \\ y_m \end{bmatrix}$$

# LMS regression with matrix derivatives

$$X\theta - y = \begin{bmatrix} x_1^T\theta \\ | \\ x_m^T\theta \end{bmatrix} - \begin{bmatrix} y_1 \\ | \\ y_m \end{bmatrix}$$

$$\frac{1}{2}(X\theta - y)^T(X\theta - y) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \theta^T x)^2$$

We want to minimize this term wrt to **θ**

# LMS regression with matrix derivatives

$$\theta = (X^T X)^{-1} X^T y$$

# Trace properties

1 • tr (a) = a

2 • trA = trA$^T$

3 • tr(A+B) = trA+trB

4 • tr(aA) = atr(A)

5 $$\nabla_A trAB = B^T$$

6 $$\nabla_{A^T} f(A) = (\nabla_A f(A))^T$$

7 $$\nabla_A trABA^TC = CAB + C^TAB^T$$

8 $$\nabla_{A^T} trABA^TC = B^TA^TC^T + BA^TC$$

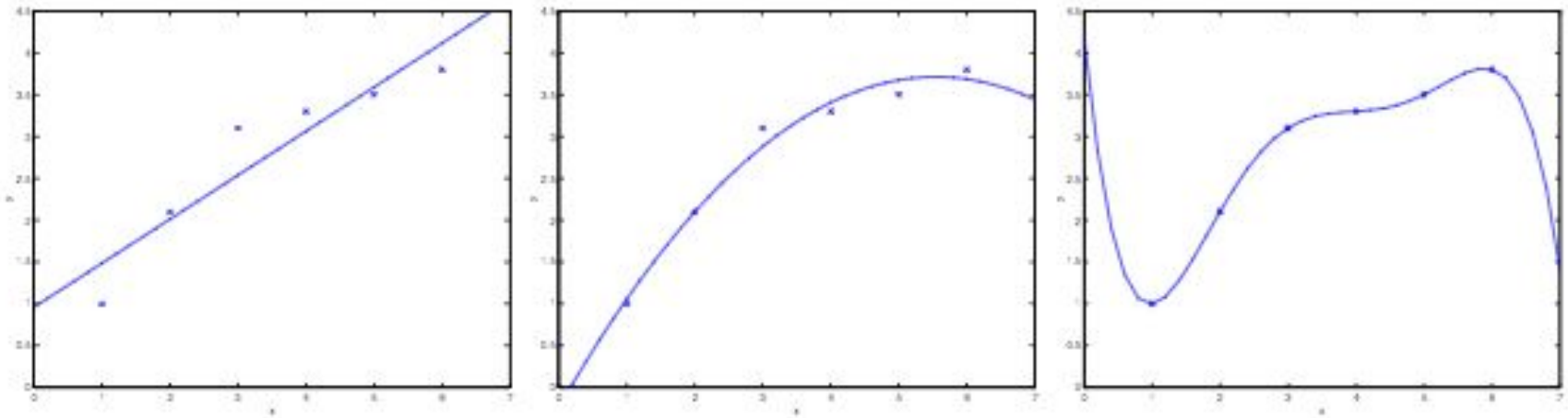
# Regression with non-linear features

- If we add extra features that are non-linear
  - For example $x^2$

| Cloth | Corn | Grass | Water | Beer | Rainfall |
|---|---|---|---|---|---|
| 4 | 6 | 3 | 10 | 0 | **76950** |
| 5 | 1 | 0 | 0 | 7 | **30234** |
| 6 | 0 | 3 | 5 | 7 | **123456** |
| 5 | 0 | 3 | 12 | 0 | **89301** |
| 4 | 3 | 0 | 6 | 7 | **?** |

- $h_{\boldsymbol{\theta}}(\mathbf{x_1}) = \theta_0 + \theta_1 x_{1,1} + \theta_2 x_{1,2} + \theta_3 x_{1,3} + \theta_4 x_{1,4} + \theta_5 x_{1,5} + \theta_6 x_{1,1}^2 + \ldots$
- These can be considered as additional features
- We can now have a line that is non-linear

# Overfitting Underfitting



Adding more non-linear features makes the line more curvy
(Adding more features also means more model parameters)

The curve can go directly to the outliers with enough parameters.
We call this effect overfitting
For the opposite case, having not enough parameters to model the data is called underfitting

# Predicting floods

| Cloth | Corn | Grass | Water | Beer | Flood? |
|---|---|---|---|---|---|
| 4 | 6 | 3 | 10 | 0 | **yes** |
| 5 | 1 | 0 | 0 | 7 | **yes** |
| 6 | 0 | 3 | 5 | 7 | **no** |
| 5 | 0 | 3 | 12 | 0 | **yes** |
| 4 | 3 | 0 | 6 | 7 | **?** |

So far we talk about predicting an amount what if we want to do classification

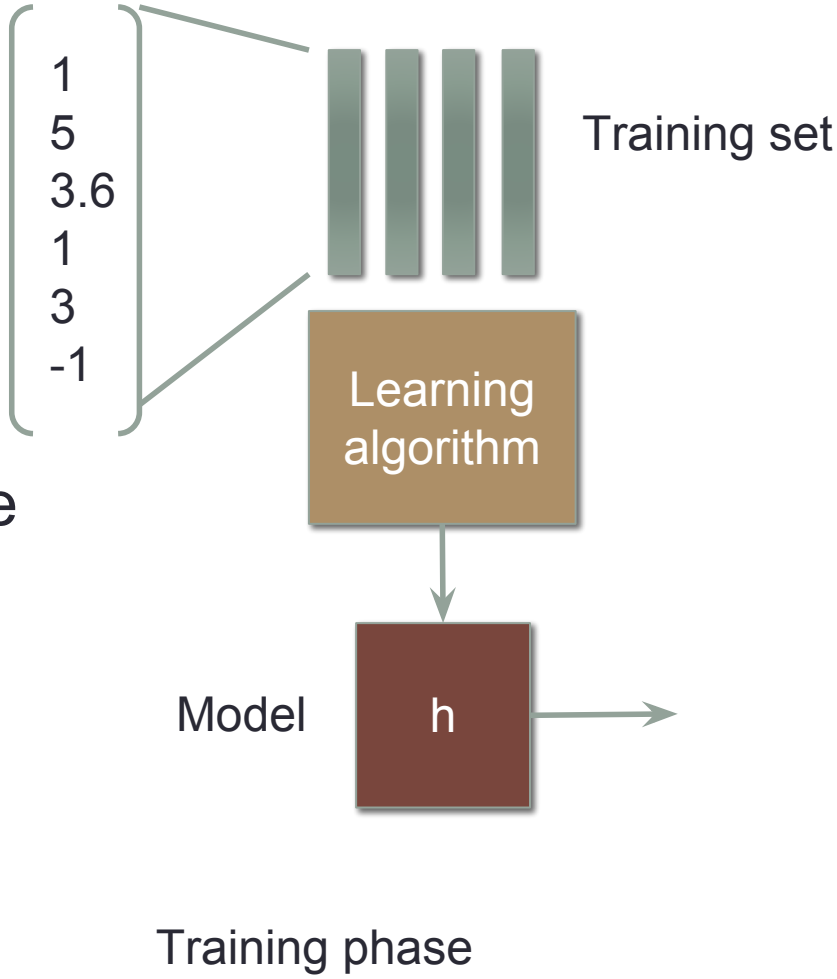
Let’s start with a binary choice. Flood or no flood

# Flood or no flood

- What would be the output?

- y = 0 if not flooded
- y = 1 if flooded

- Anything in between is a score for how likely it is to flood



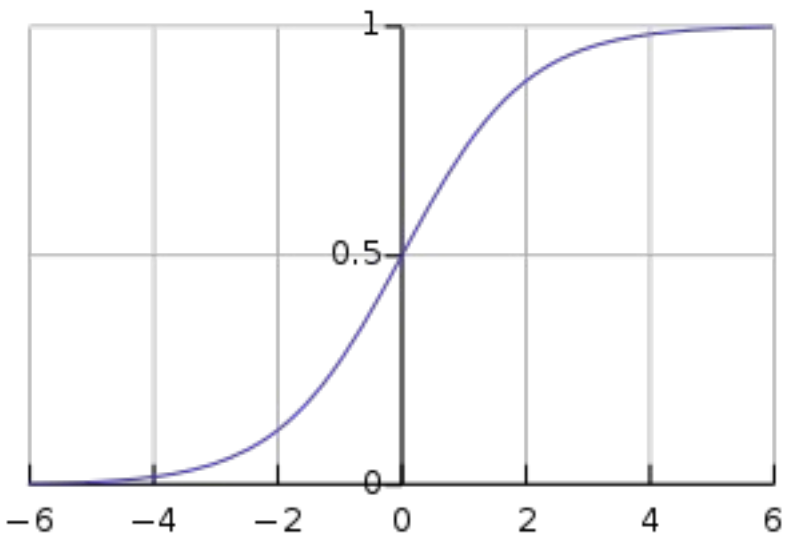
# Can we use regression?

- Yes
- $h_{\boldsymbol{\theta}}(\mathbf{x_1}) = \theta_0 + \theta_1 x_{1,1} + \theta_2 x_{1,2} + \theta_3 x_{1,3} + \theta_4 x_{1,4} + \theta_5 x_{1,5}$

- But
- What does it mean when h is higher than 1?
- Can h be negative? What does it mean to have a negative flood value?

# Logistic function

- Let's force h to be between 0 and 1 somehow
- Introducing the logistic function (sigmoid function)




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

https://en.wikipedia.org/wiki/Logistic_function

# Logistic Regression

- Pass $\theta^T \mathbf{x}$ through the logistic function

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

# Loss function?

- MSE error no longer a good candidate

# Logistic Regression update rule

$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - h_\theta(x_i))x_i^{(j)}$$

Update rule for linear regression

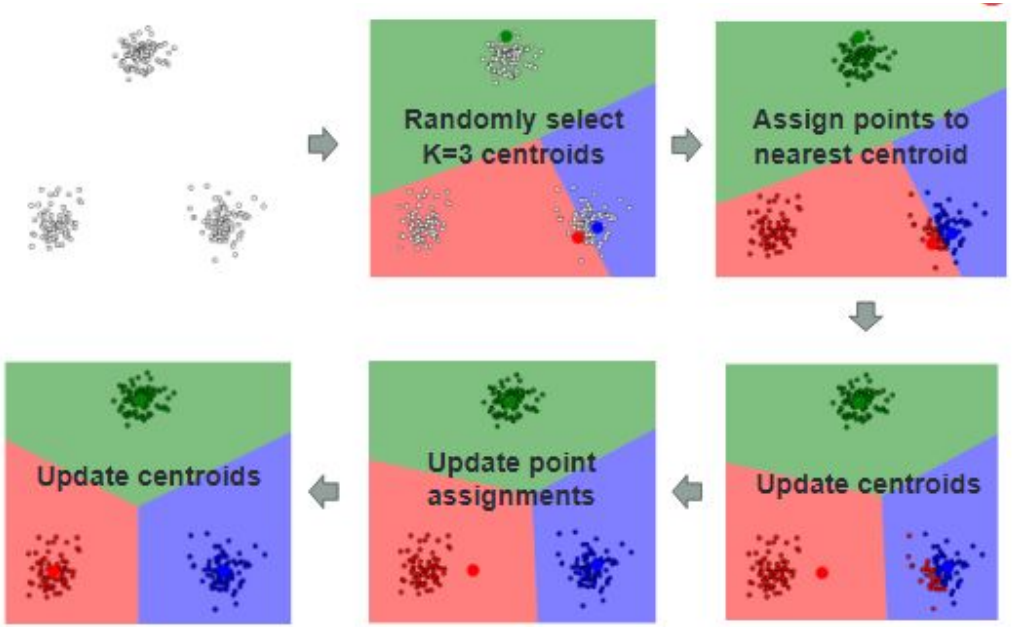
$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

# Summary

KNN

K-mean clustering

Iterative method




For linear regression, direct or iterative should yield similar answers as long as the learning rate is small enough (No local minima to get stuck - Convex problem)

Regression

Minimizing a loss function

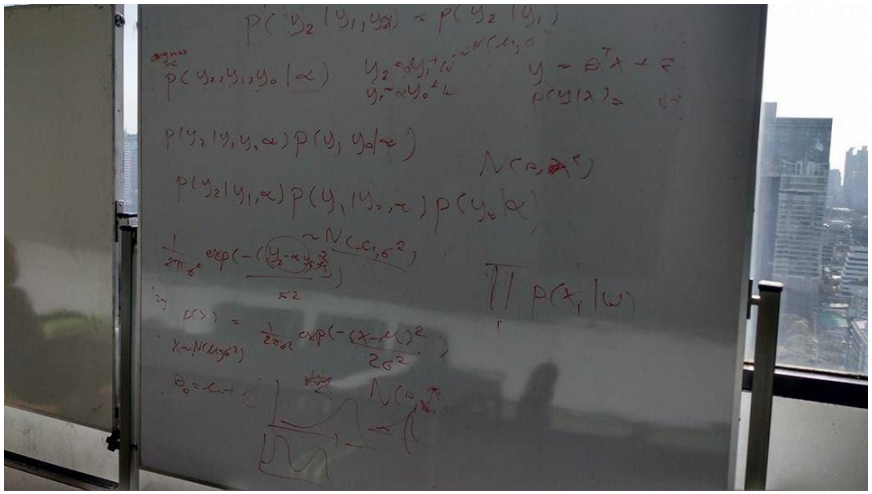
Solve directly vs Iterative (gradient descent)

$$\theta = (X^T X)^{-1} X^T y$$

$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

# Homework

Some matrix, some K-mean, and some regression

# Office hours

- Wednesdays 16.30-18.00 starting from Aug 22nd
- 29th moved to 31st
- Location Sky Cafe