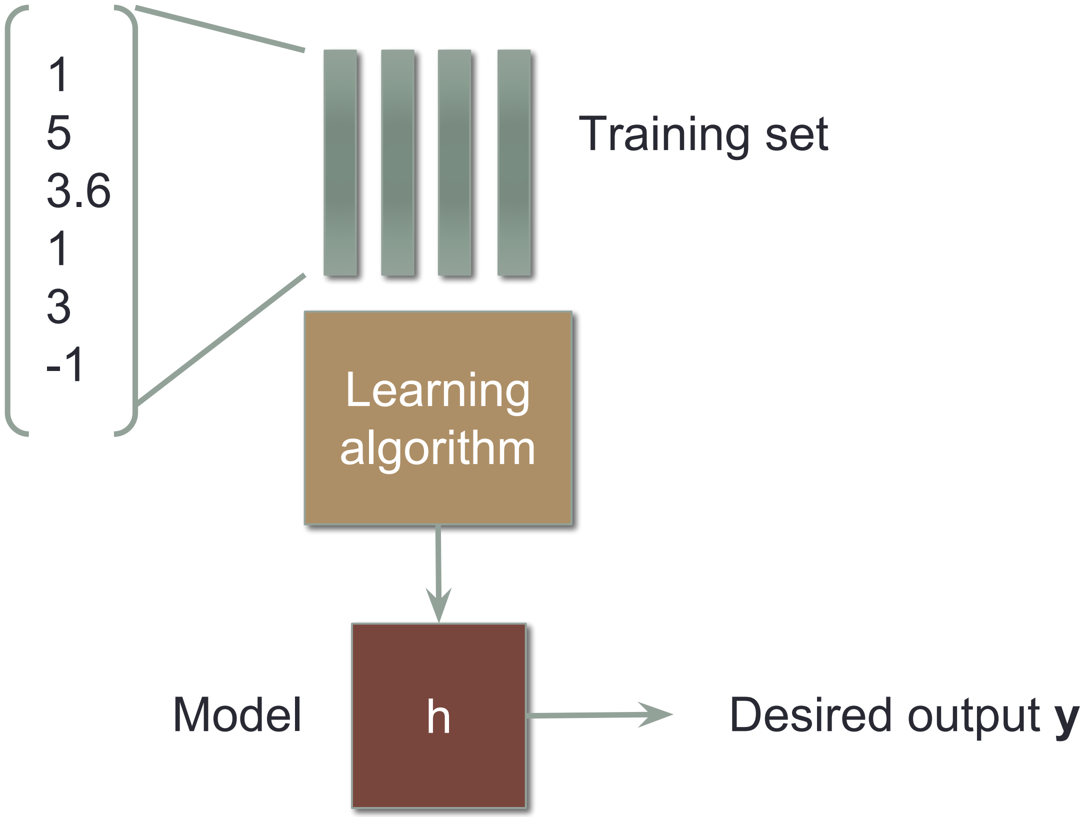
REGRESSION

with some K-mean clustering

How do we learn from data?



$$\begin{bmatrix}1\\5\\3.6\\1\\3\\-1\end{bmatrix}$$

Training set

Learning algorithm

Model

h

Desired output **y**

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

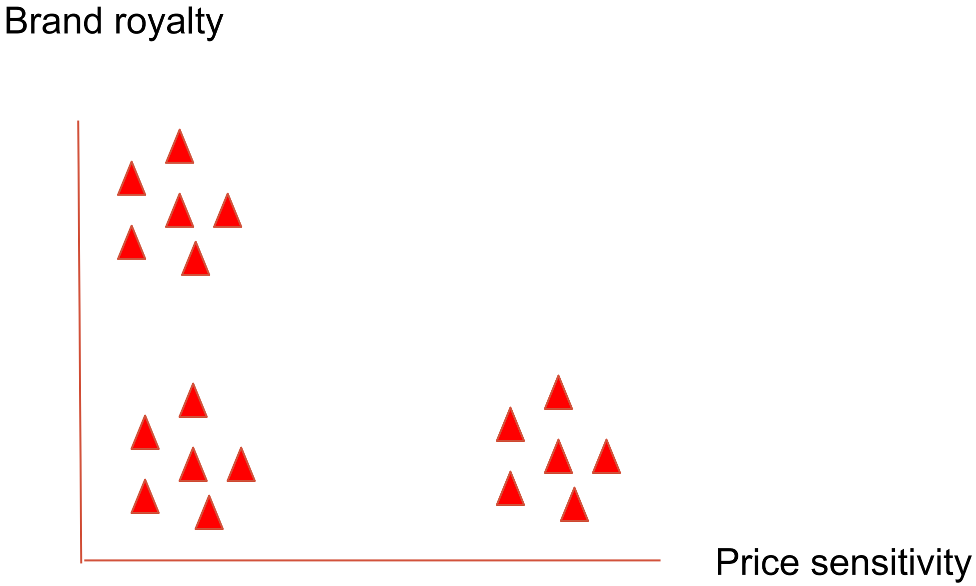
   Train an agent to take appropriate actions in an environment by maximizing rewards

Our first model - Unsupervised learning

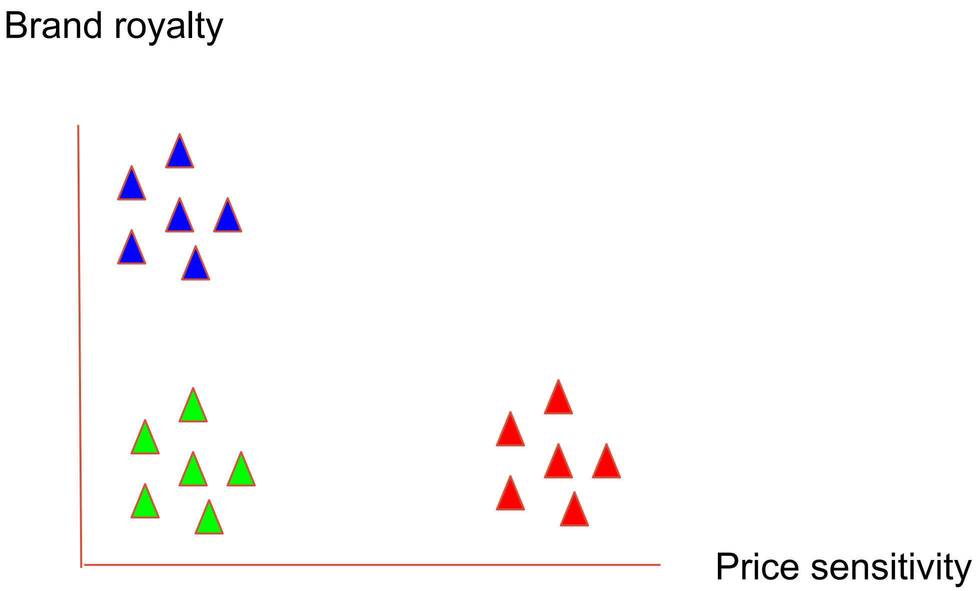
Discover the hidden structure in unlabeled data X (no y)

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

Example - Customer analysis

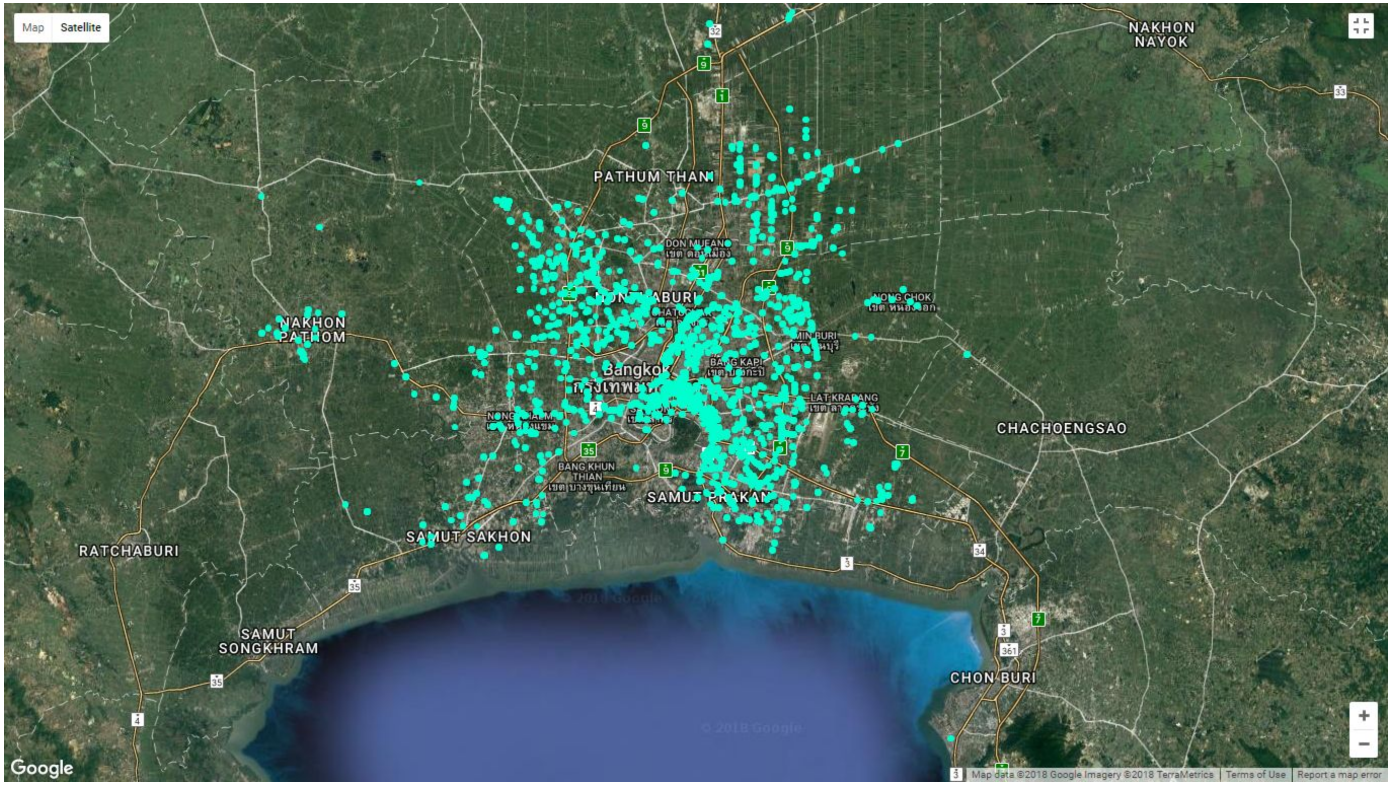


Example - Customer analysis



Example - Real Estate segmentation in Thailand

What should be the input feature of this?



Example - Real Estate segmentation in Thailand

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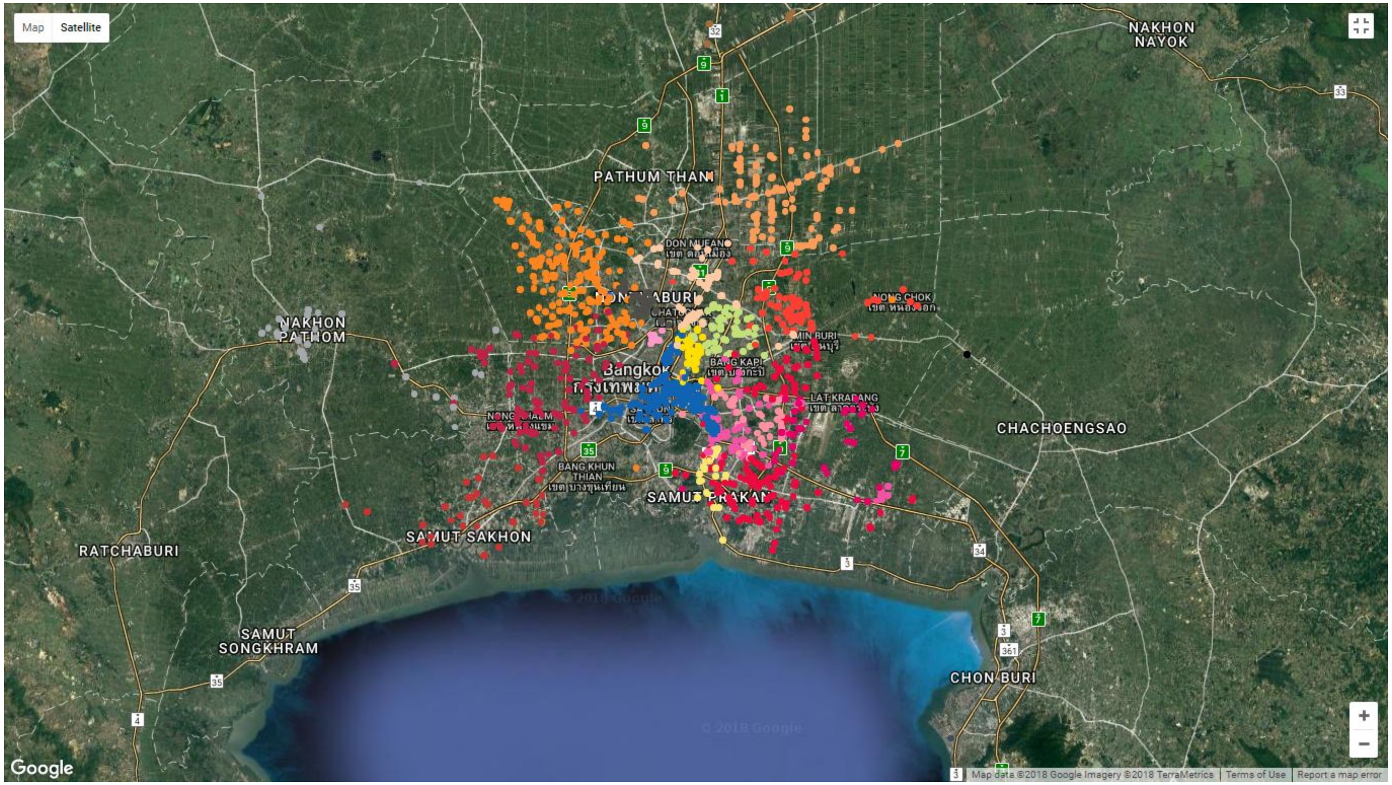
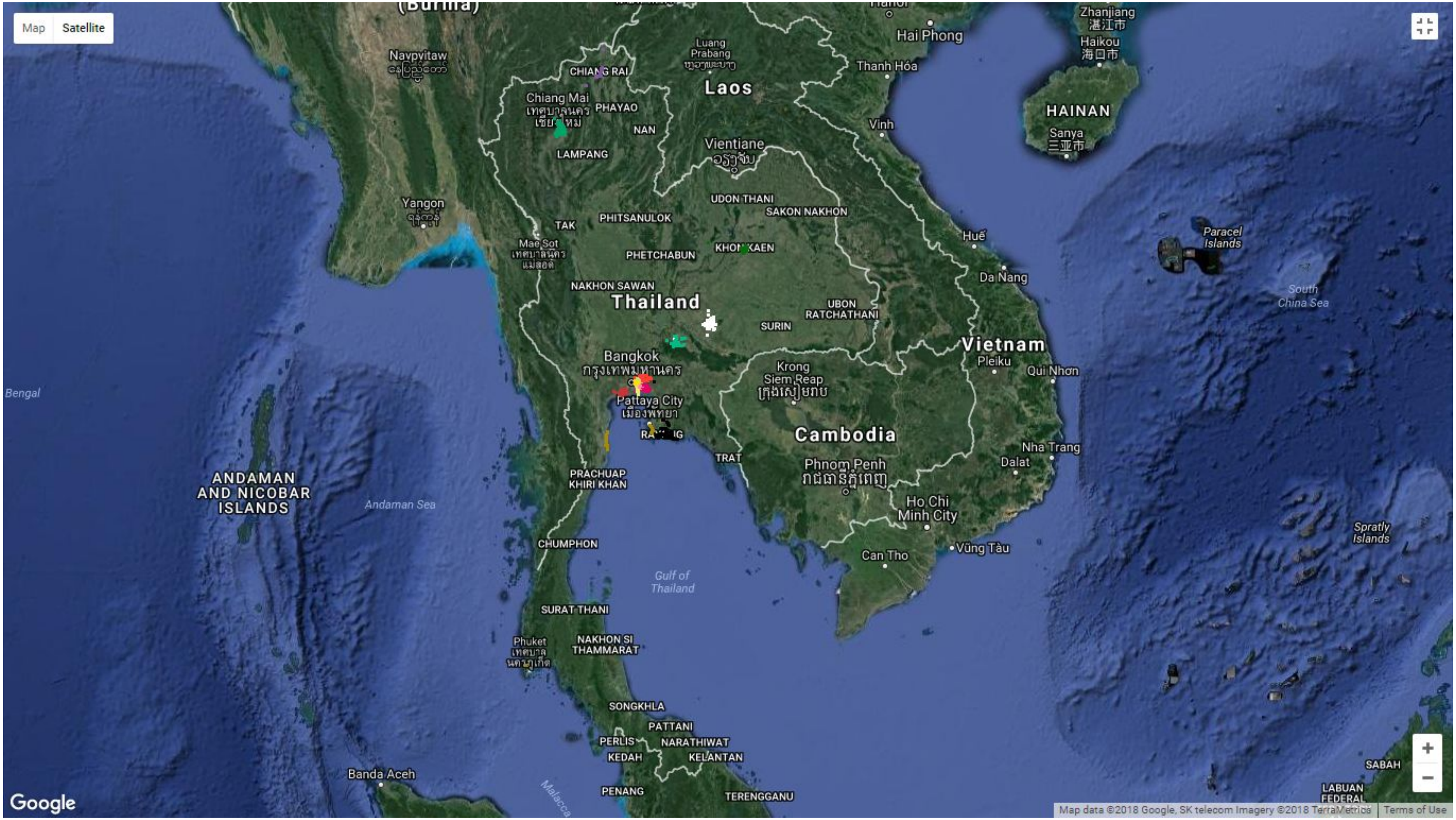
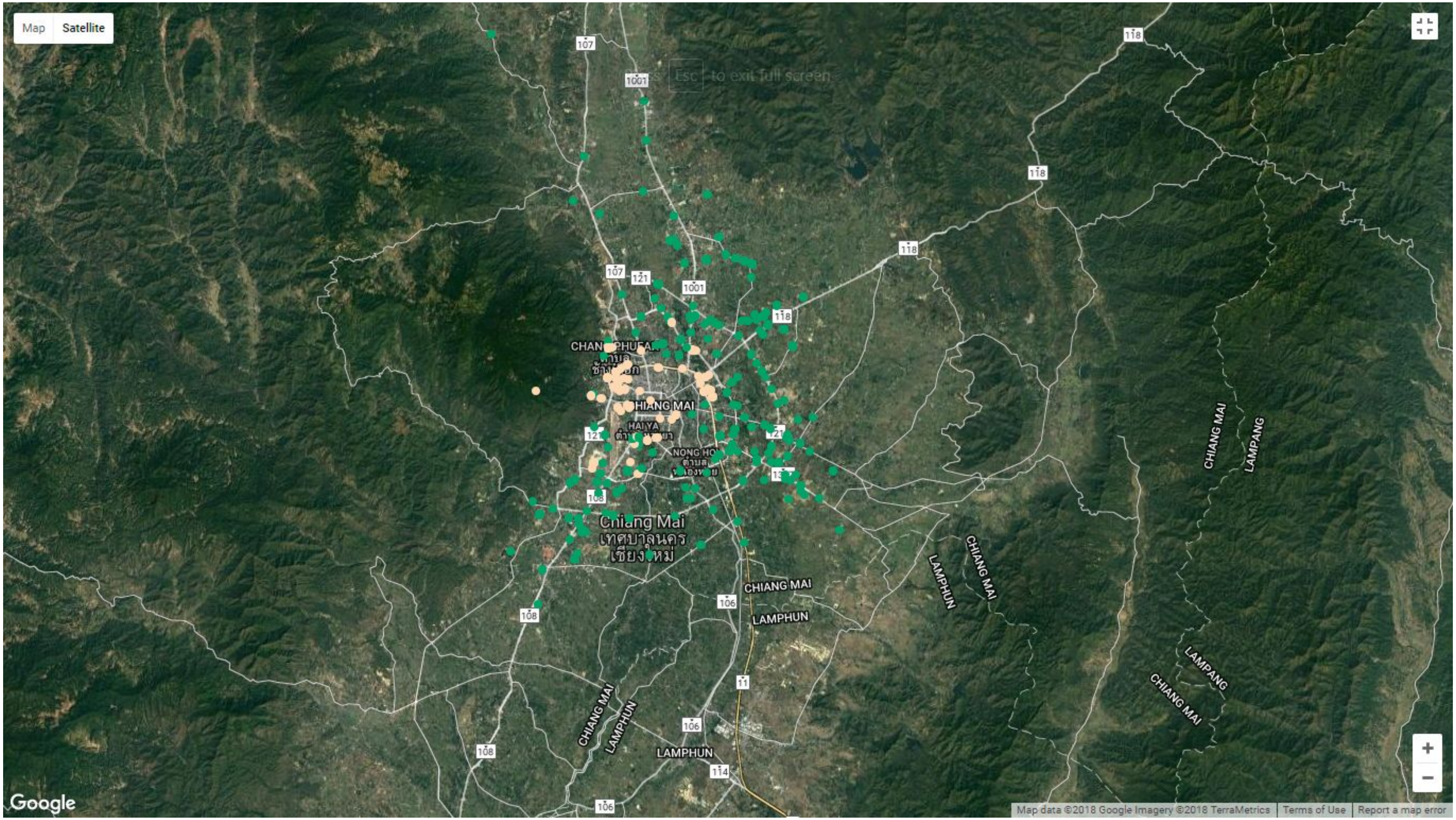


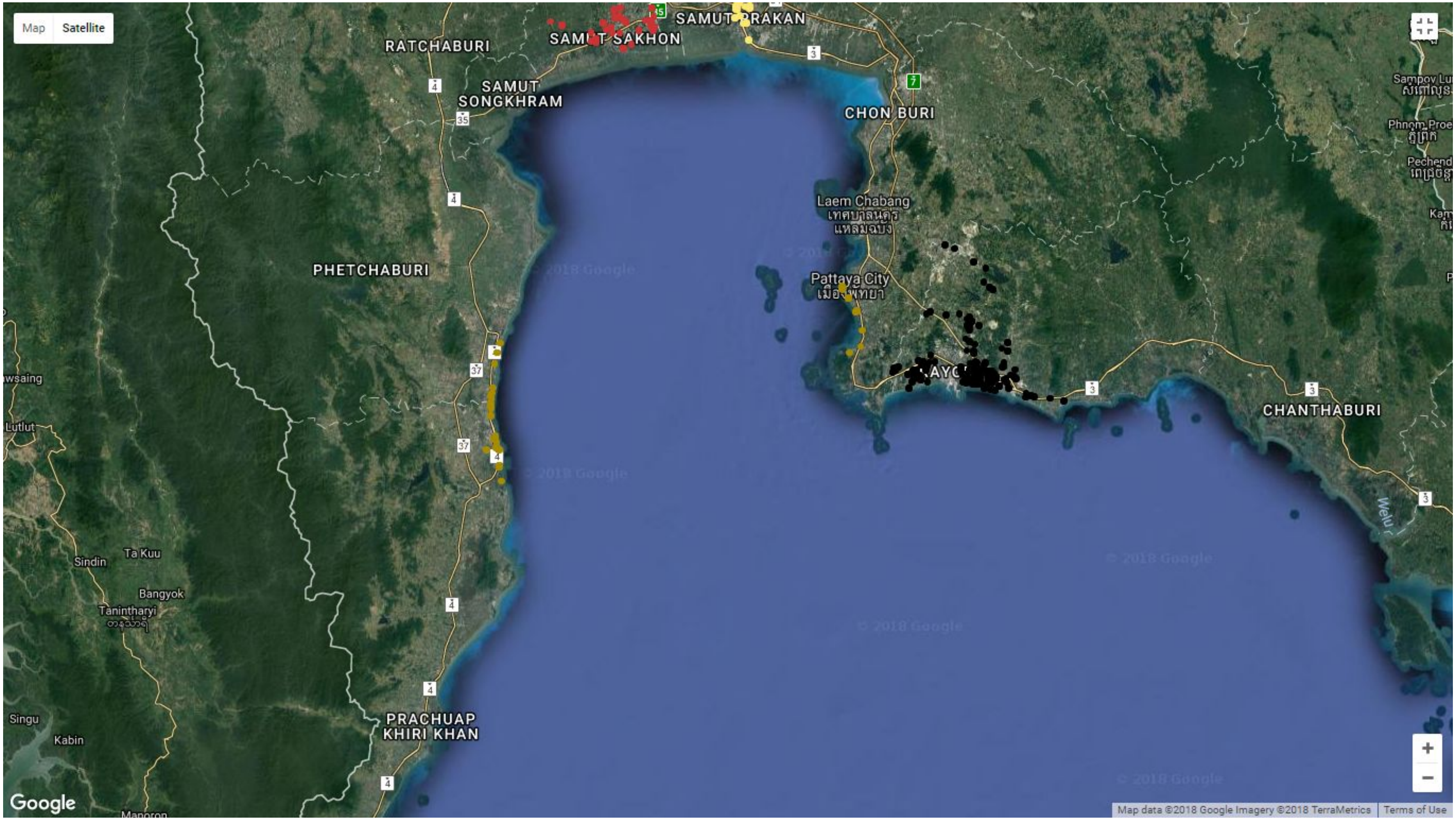
Example - Real Estate segmentation in Thailand



Example - Real Estate segmentation in Thailand



Example - Real Estate segmentation in Thailand



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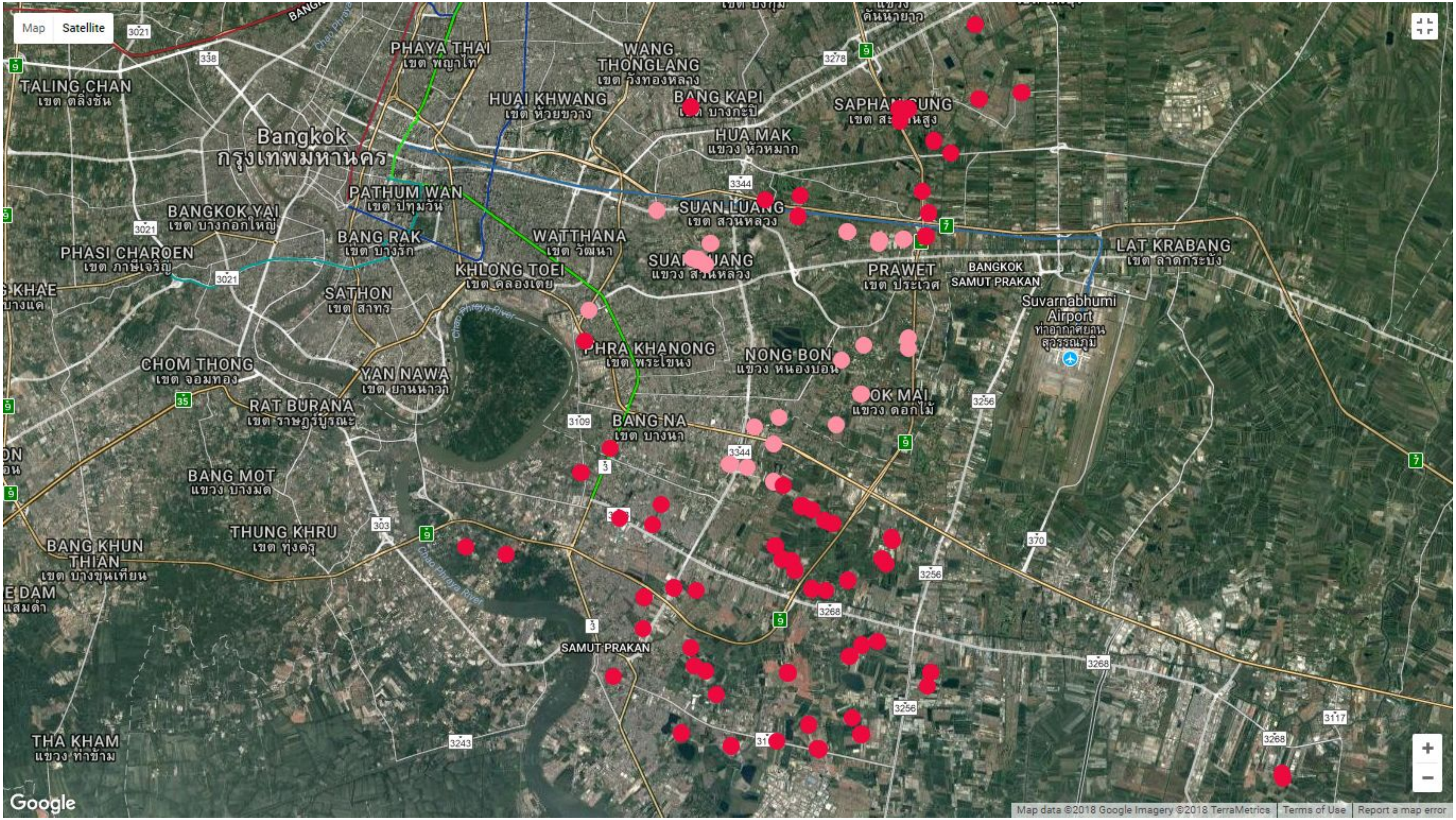
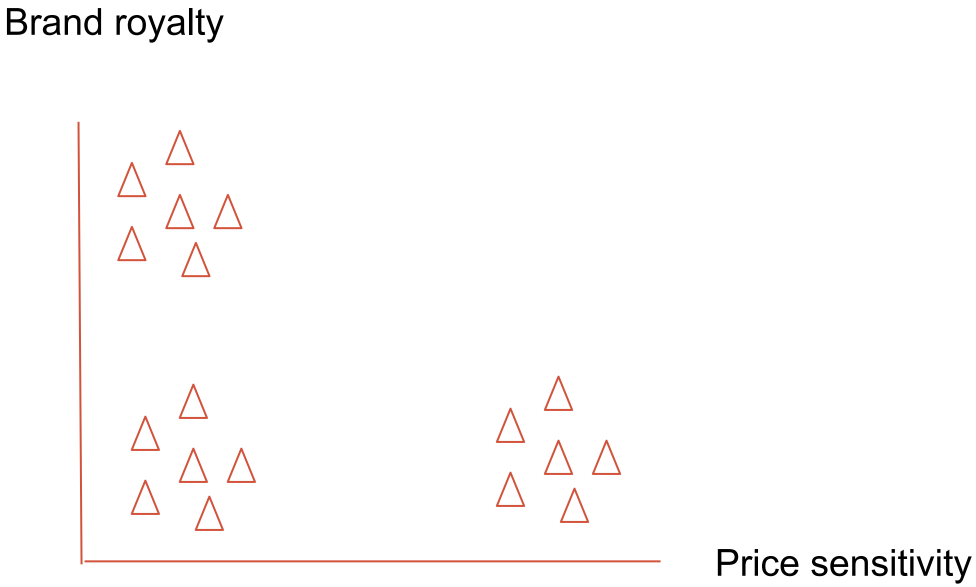


K-mean clustering

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

Too hard…



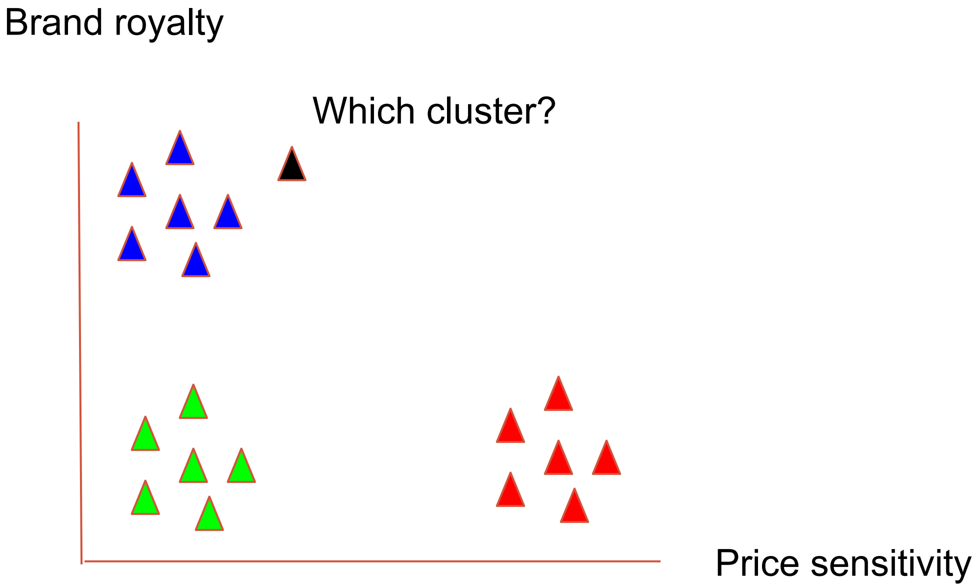
K-mean clustering

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

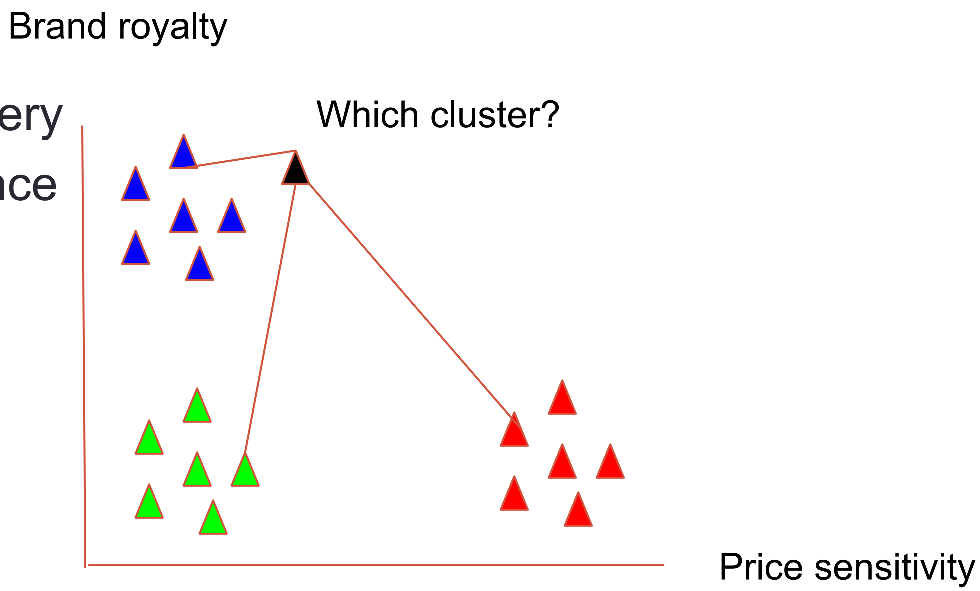
Find the closest training data, assign the same label as the training data

Given query data

For every point in the training data

    Compute the distance with the query

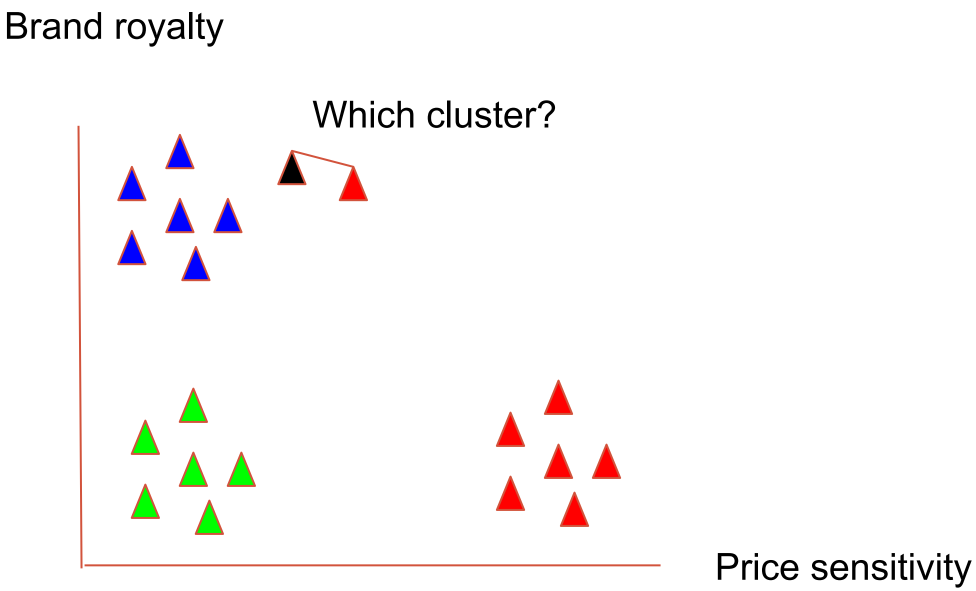
    Assign label of the smallest distance



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

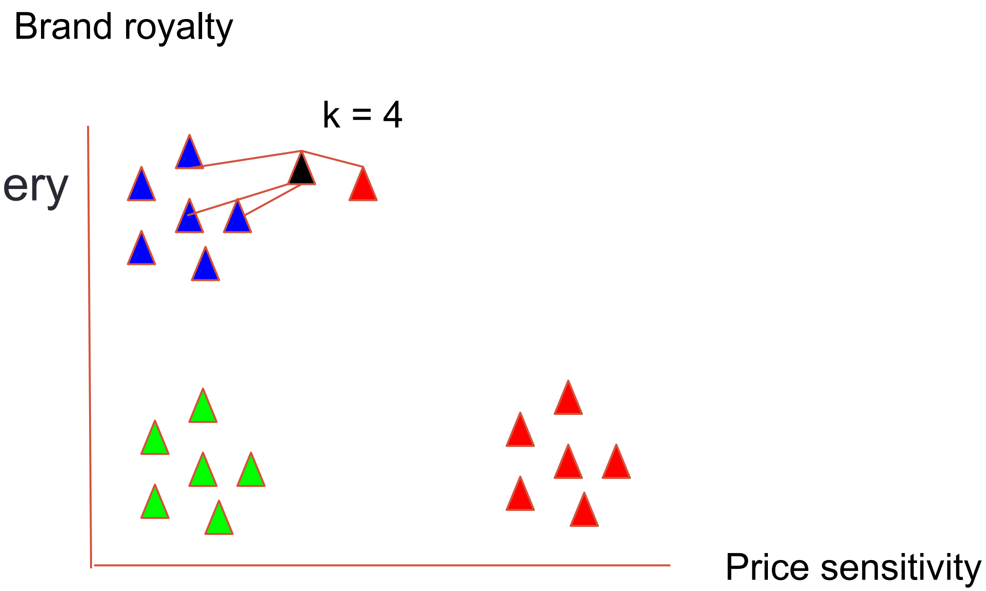
Given query data

For every point in the training data

    Compute the distance with the query

    Find the K closest data points

    Assign label by voting



K-Nearest Neighbour (kNN) classification

Nearest Neighbour is susceptible to noise in the training data

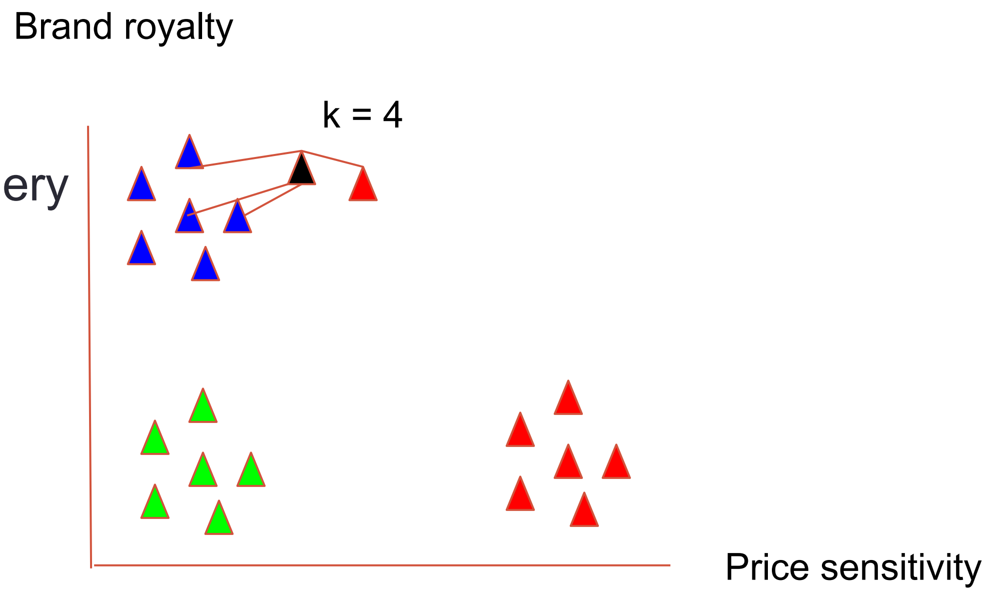
Use a voting scheme instead

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

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



Closest?

We need some kind of distance or similarity measures

F(**X**$_1$,**X**$_2$) = d

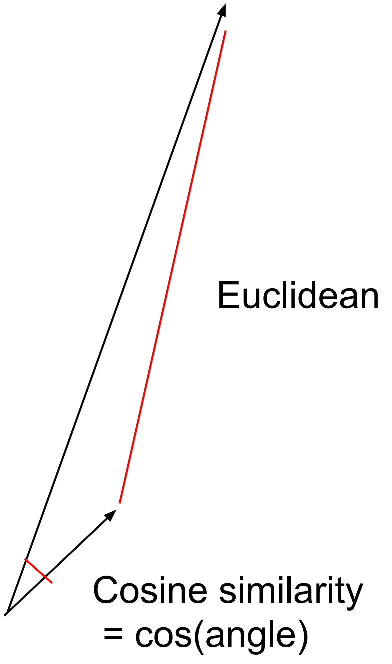
$$X_1 = [x_{1,1}, x_{1,2}, \ldots, x_{1,n}]$$

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

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

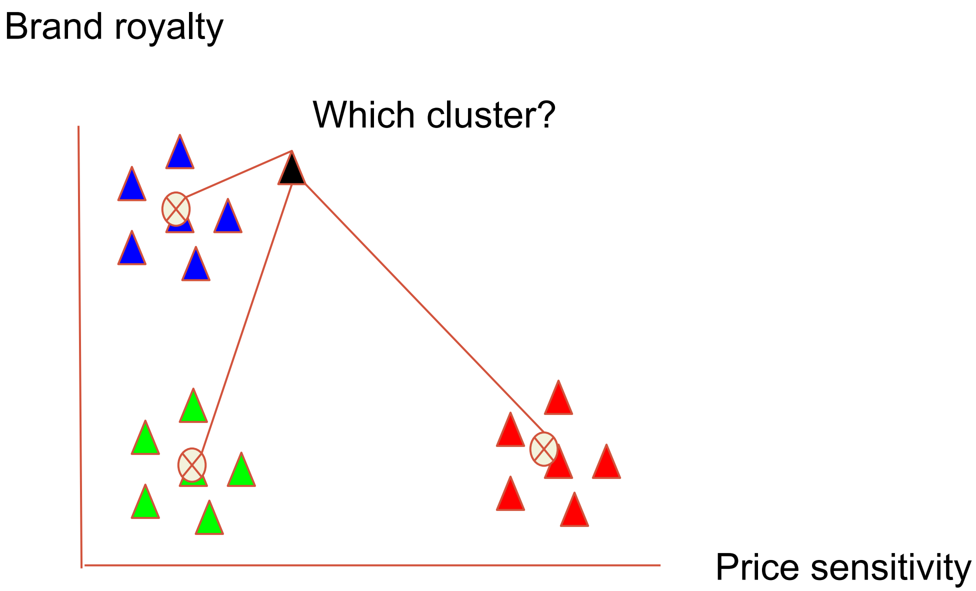
Basically the representative of the cluster

Find the mean location of the cluster by averaging

Can use mode or median depending on the data

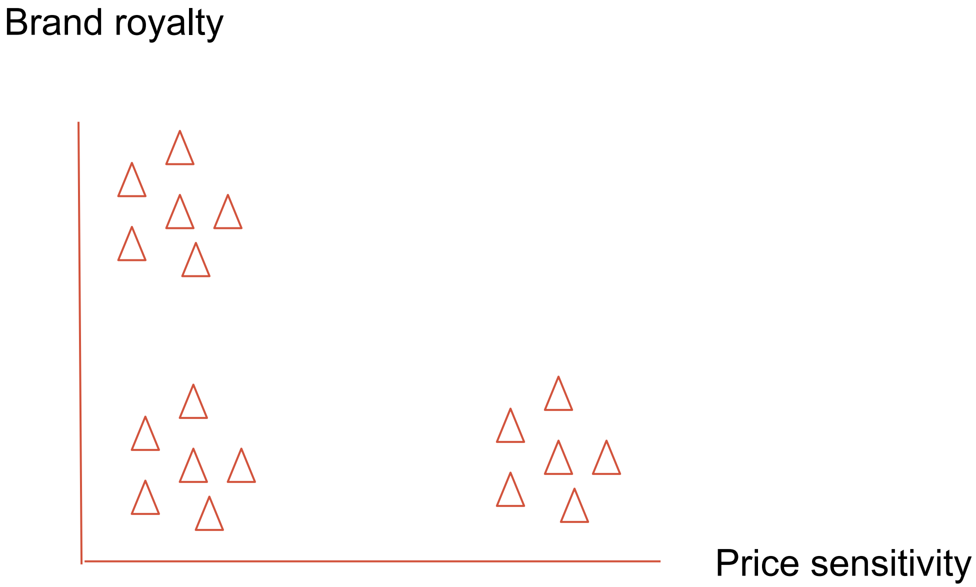
O(JL)

L - number of clusters

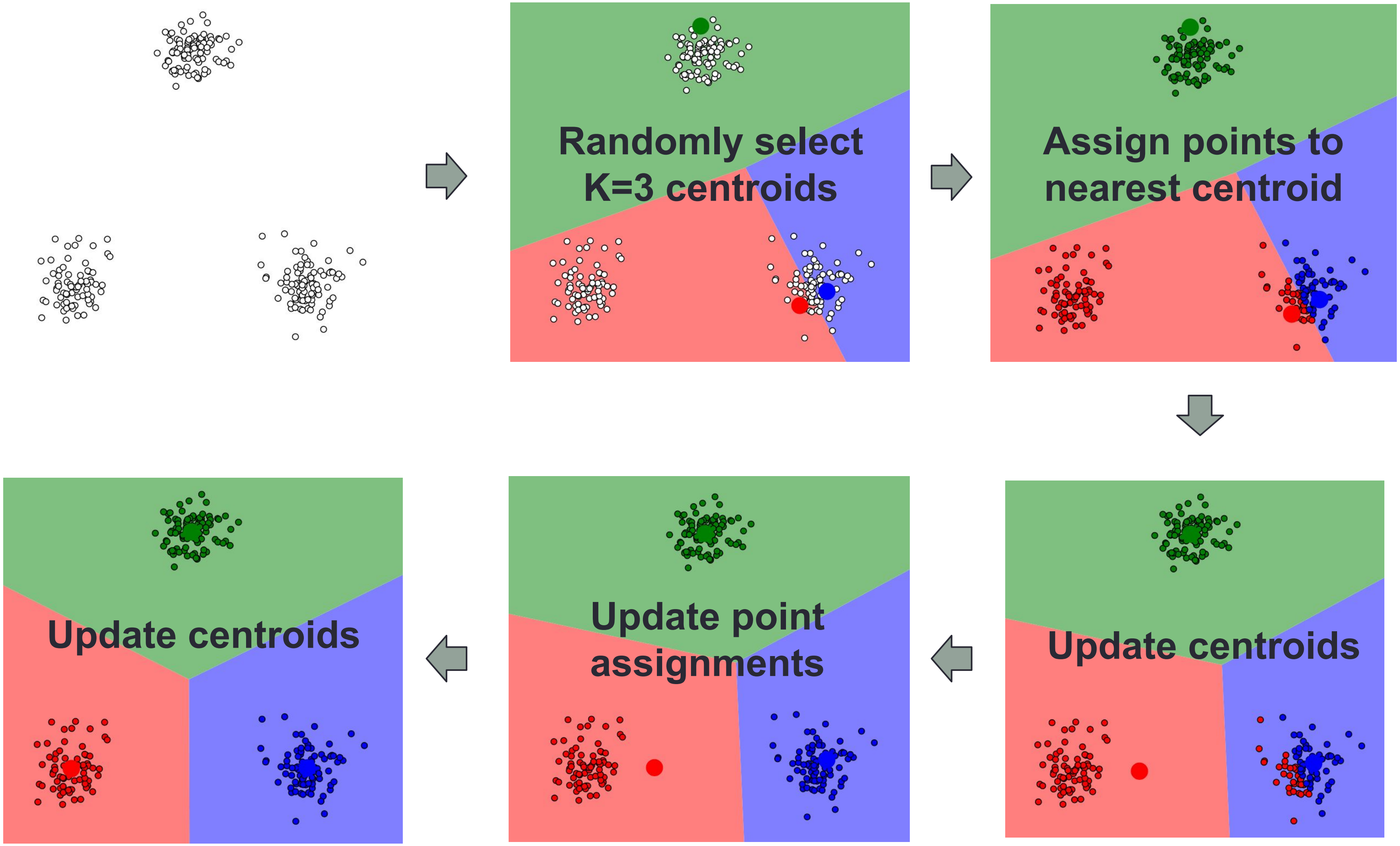


K-mean clustering

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



Randomly select K=3 centroids

Assign points to nearest centroid

Update centroids

Update point assignments

Update centroids

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.

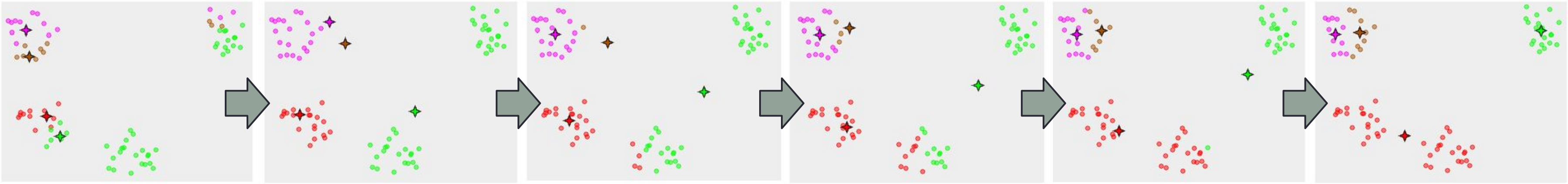
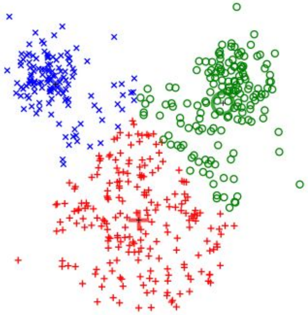
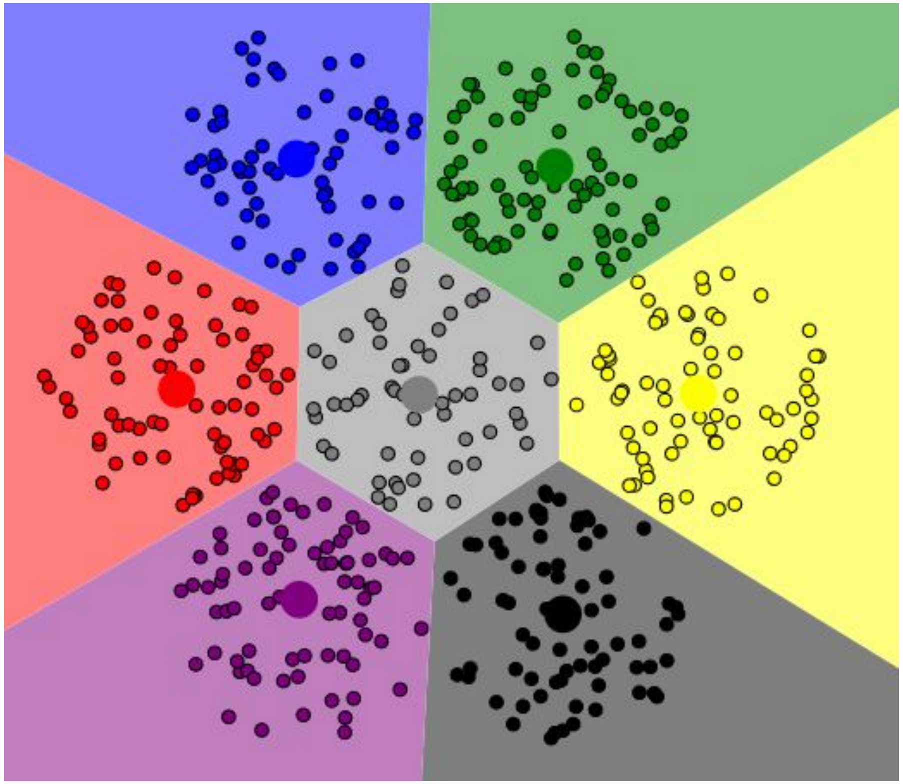


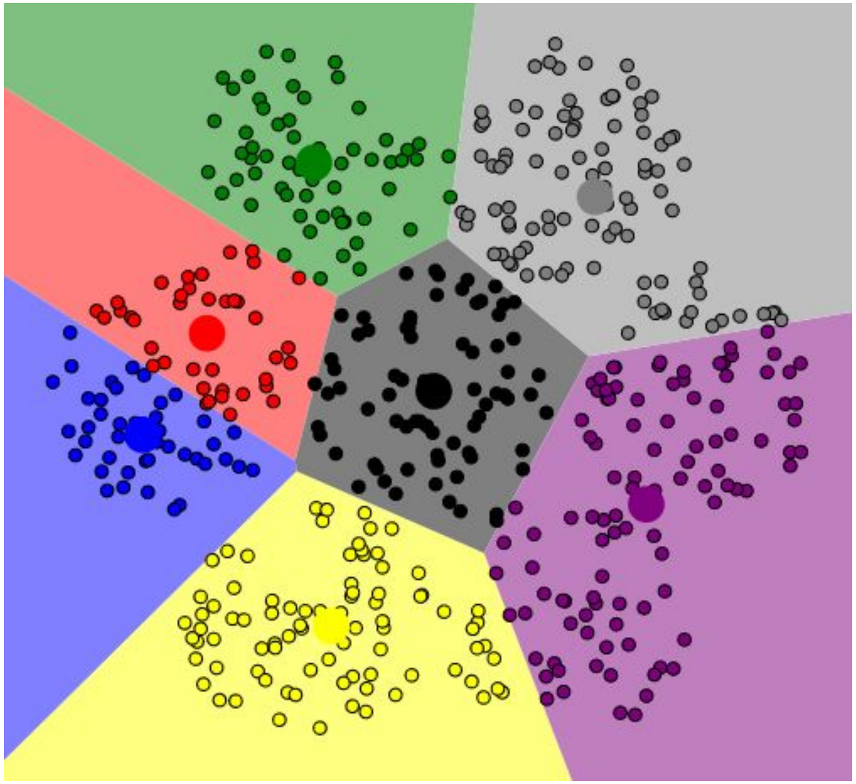
Image from https://en.wikipedia.org/wiki/K-means_clustering

- 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

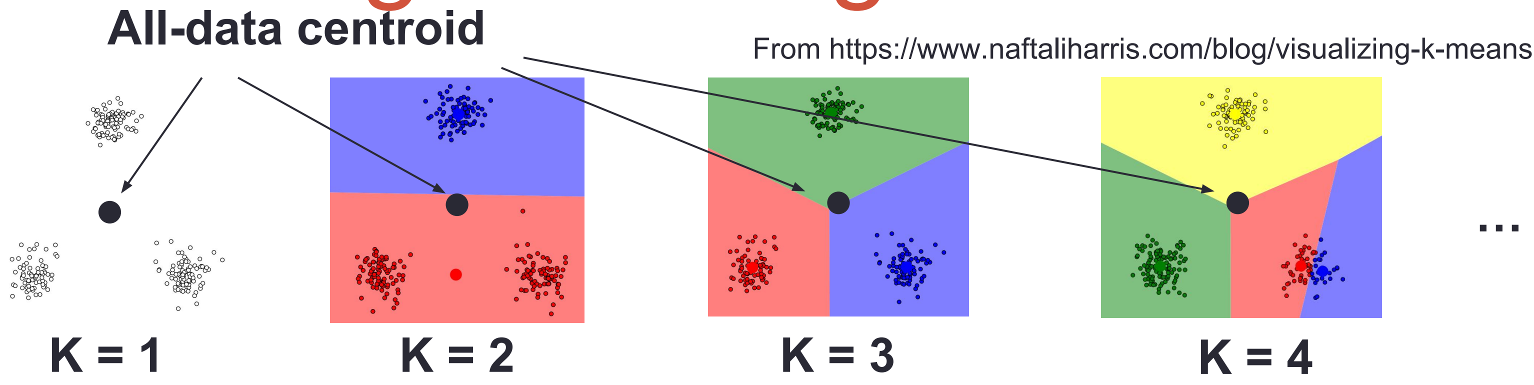




Solution, try different randomization and pick the best

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

Selecting K - Using Elbow method



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

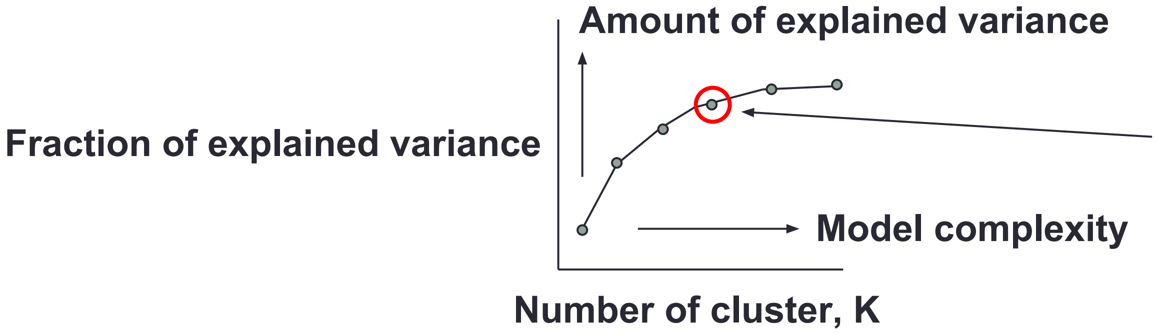
$$\text{fraction of explained variance} = \frac{\text{between-cluster variance}}{\text{all-data variance}}$$

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

M_i = centroid of ith cluster, and

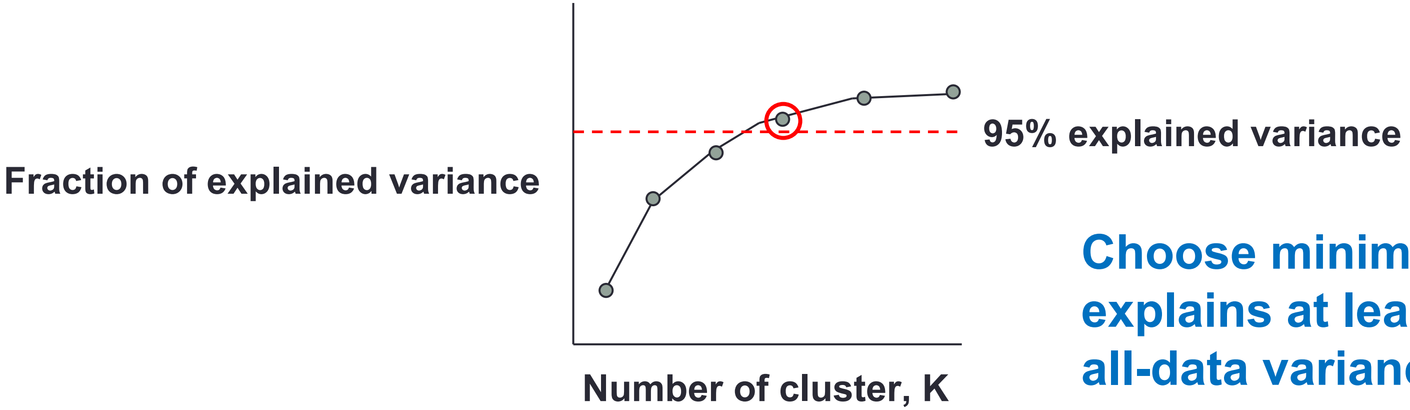
M = all-data centroid.

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

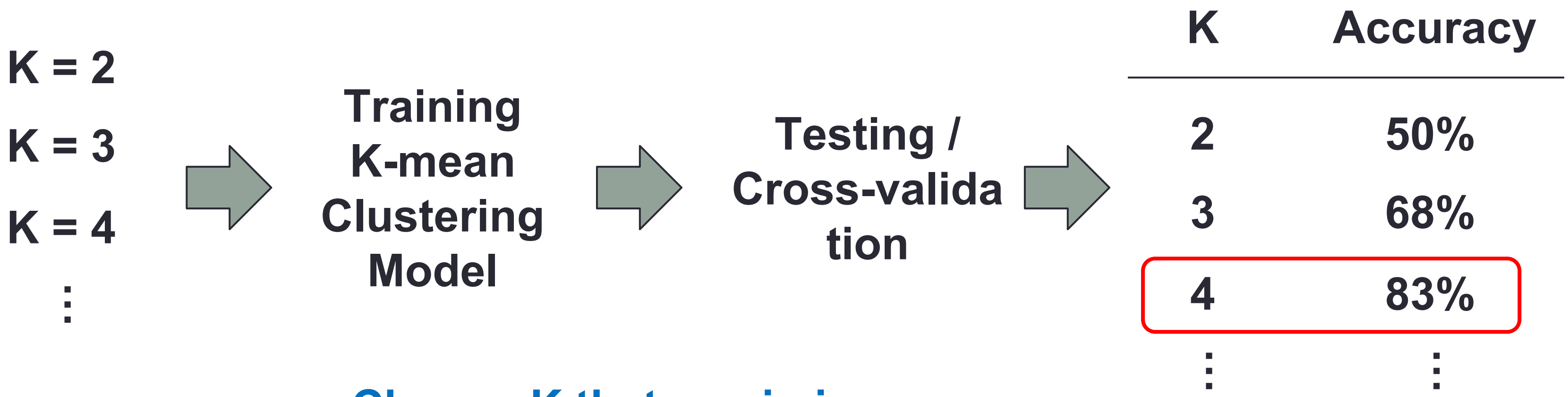


The elbow method chooses K where increasing complexity doesn't yield much in return.

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

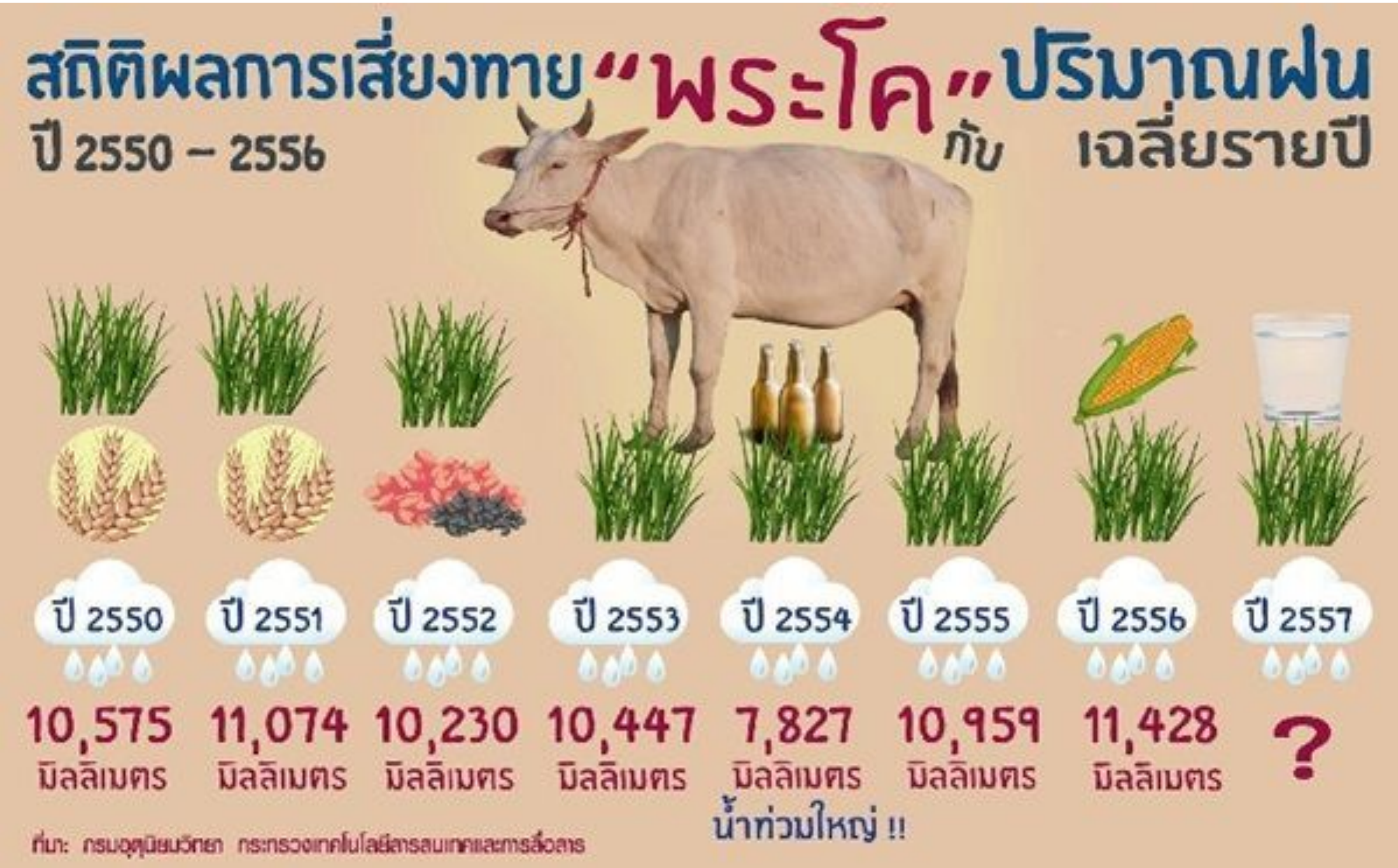
REGRESSION

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	**?**

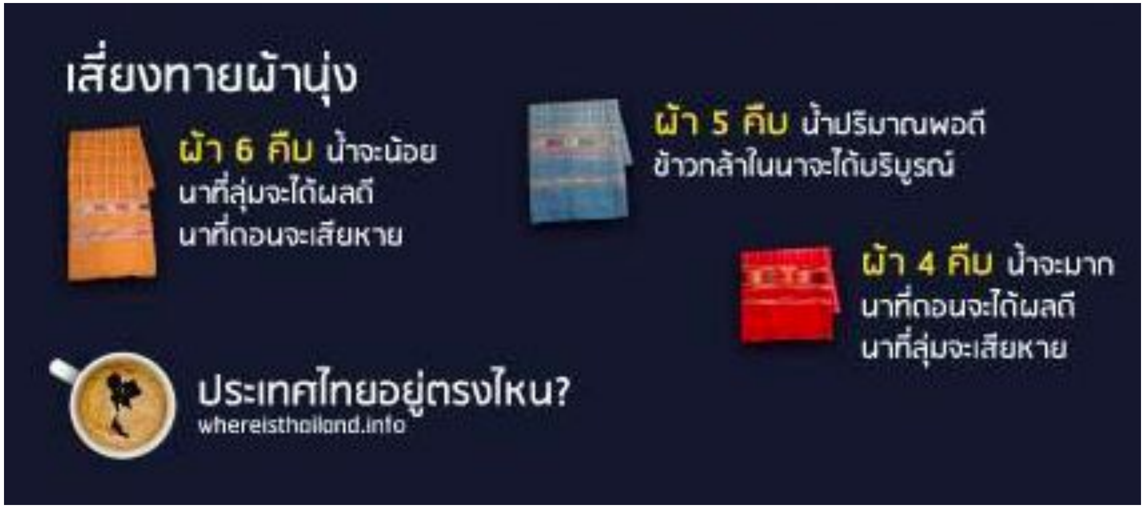
We assume the input features have some correlation with the amount of rainfall.

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



เสี่ยงทายผ้านุ่ง

ผ้า 6 คืบ น้ำจะน้อย
นาที่ลุ่มจะได้ผลดี
นาที่ดอนจะเสียหาย

ผ้า 5 คืบ น้ำปริมาณพอดี
ข้าวกล้าในนาจะได้บริบูรณ์

ผ้า 4 คืบ น้ำจะมาก
นาที่ดอนจะได้ผลดี
นาที่ลุ่มจะเสียหาย

ประเทศไทยอยู่ตรงไหน?
whereisthailand.info

Predicting the amount of rainfall

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

  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

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

- θs are the parameter (or weights)

Assume x_0 is always 1

- 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 θ

- 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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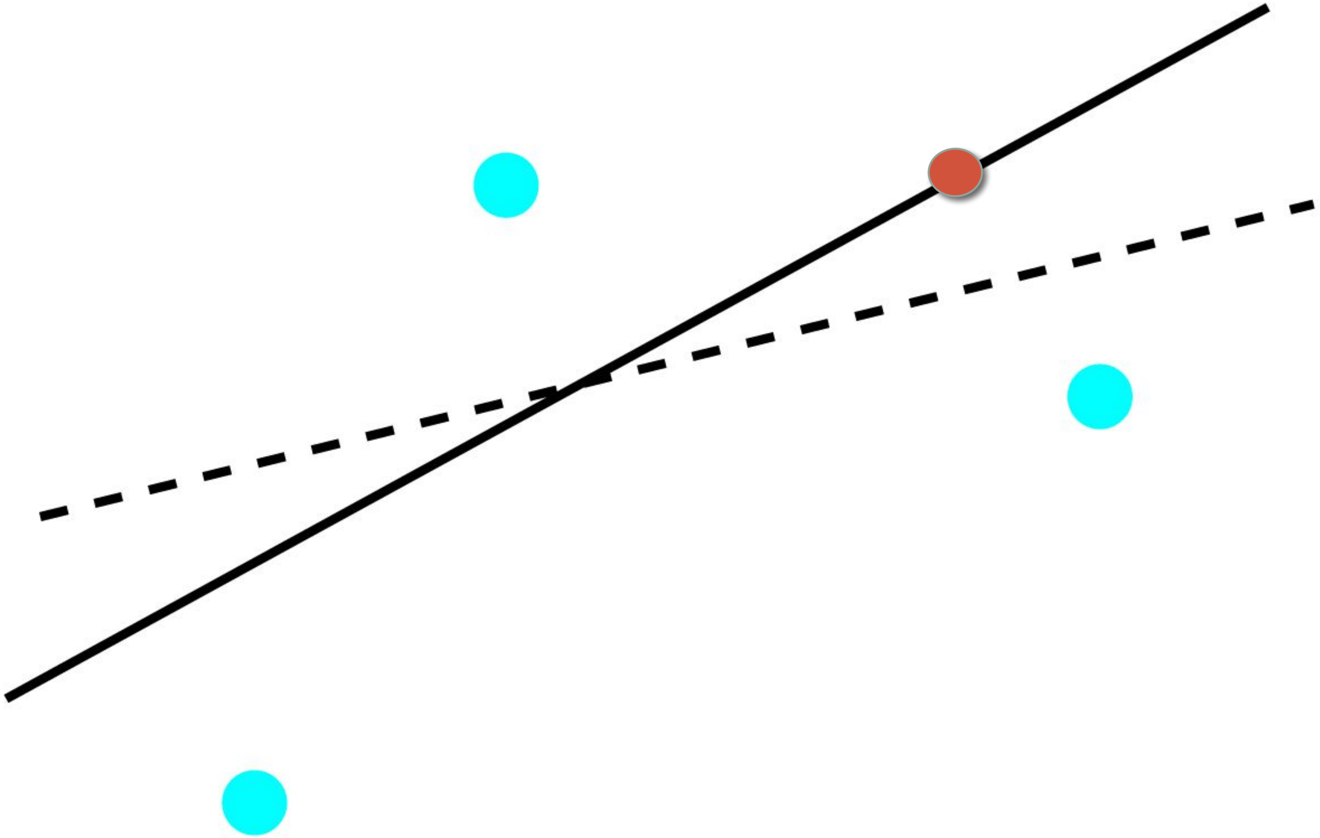

https://chem.libretexts.org/Textbook_Maps/Analytical_Chemistry_Textbook_Maps/Map%3A_Analytical_Chemistry_2.0_(Harvey)/05_Standardizing_Analytical_Methods/5.4%3A_Linear_Regression_and_Calibration_Curves

Cost function (Loss function)

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

m is the number of training examples

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

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

i here is the index of the training example

Note how **x** is bolded

Cost function (Loss function)

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

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

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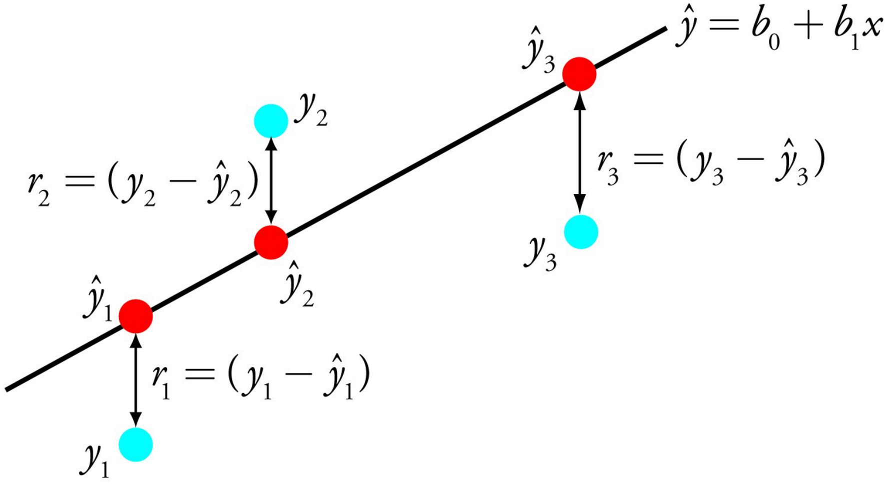

$\hat{y} = b_0 + b_1 x$
$\hat{y}_3$
y_2
$r_2 = (y_2 - \hat{y}_2)$
$r_3 = (y_3 - \hat{y}_3)$
y_3
$\hat{y}_2$
$\hat{y}_1$
$r_1 = (y_1 - \hat{y}_1)$
y_1

Cost function (Loss function)

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

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

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

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

Picking θ

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

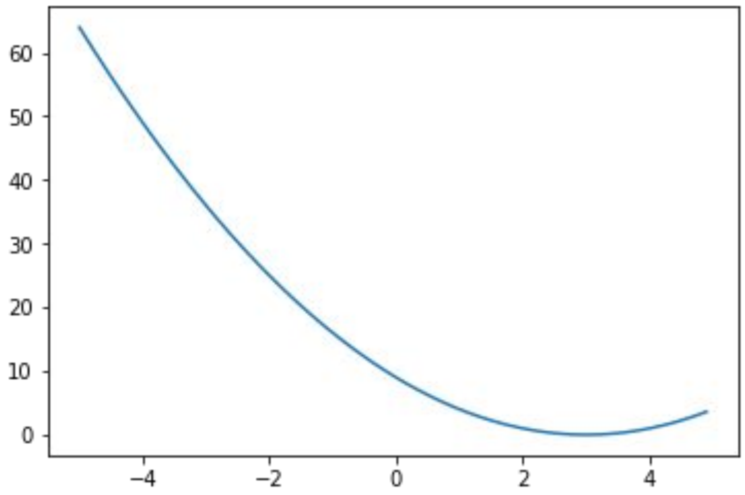
- How to quantify best performance?

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

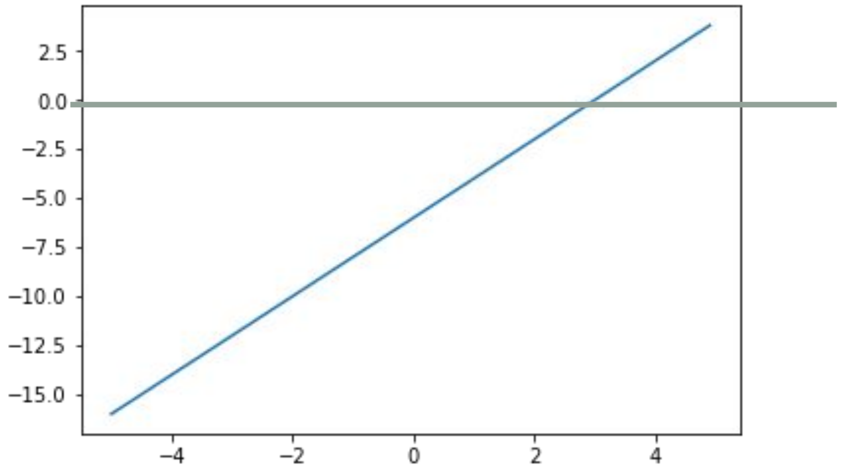
Minimizing a function

- 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



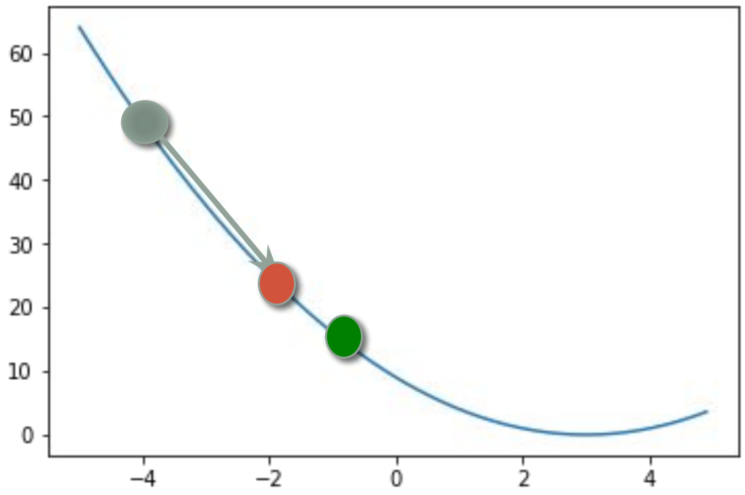
y



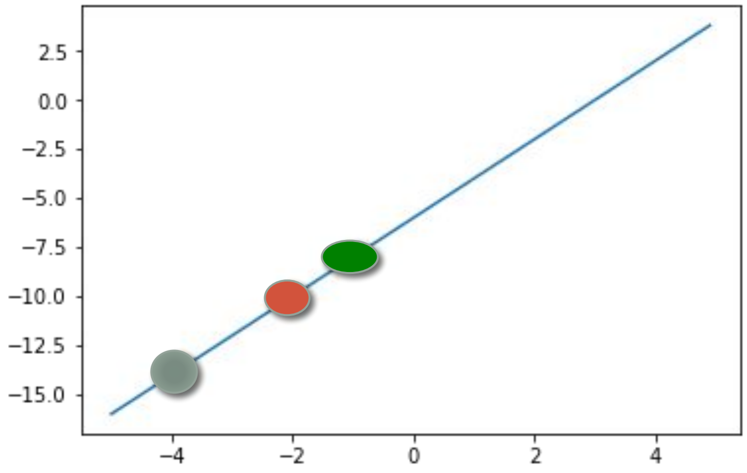
dy/dx

First what does dy/dx means?

Gradient descent



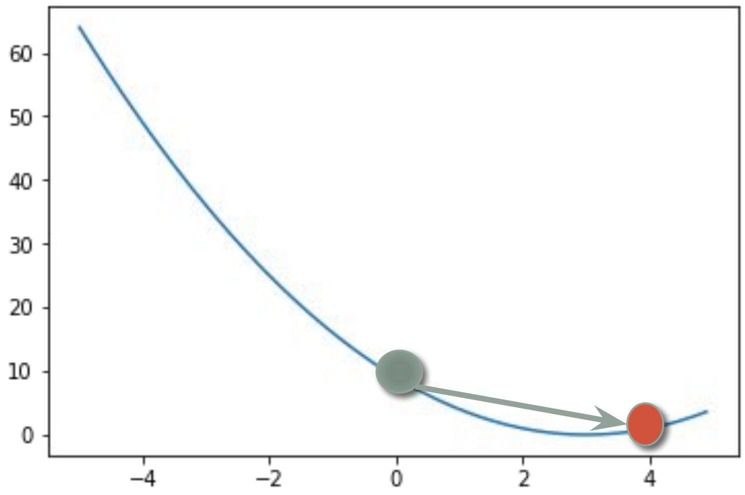
y



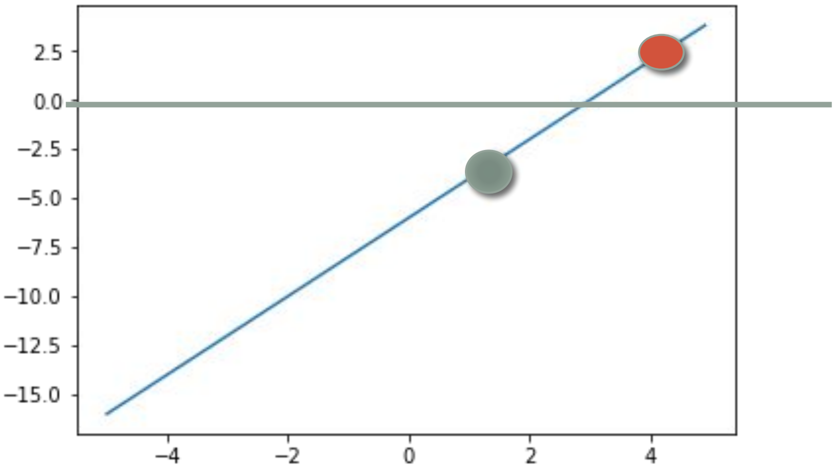
dy/dx

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

Gradient descent



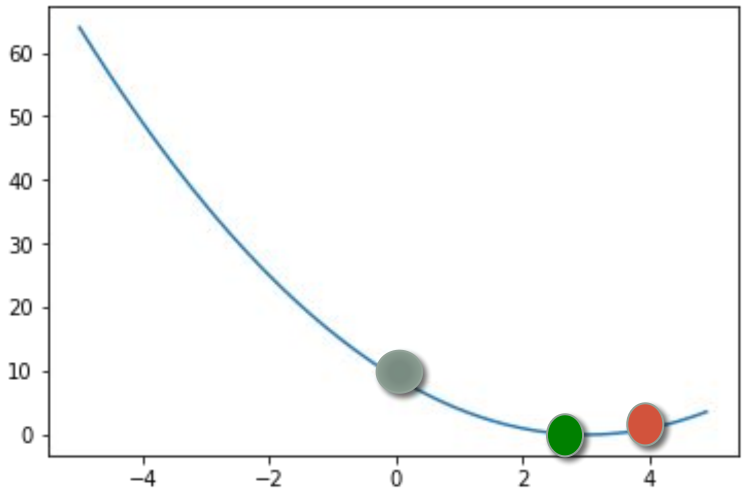
y



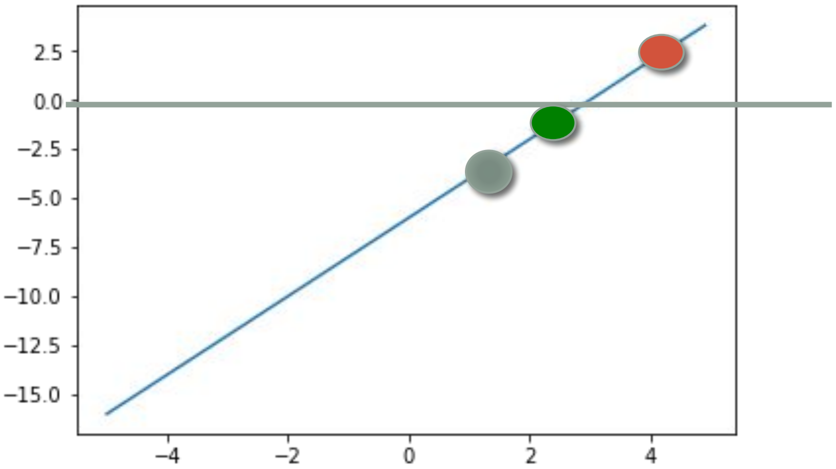
dy/dx

What happens when you overstep?

Gradient descent



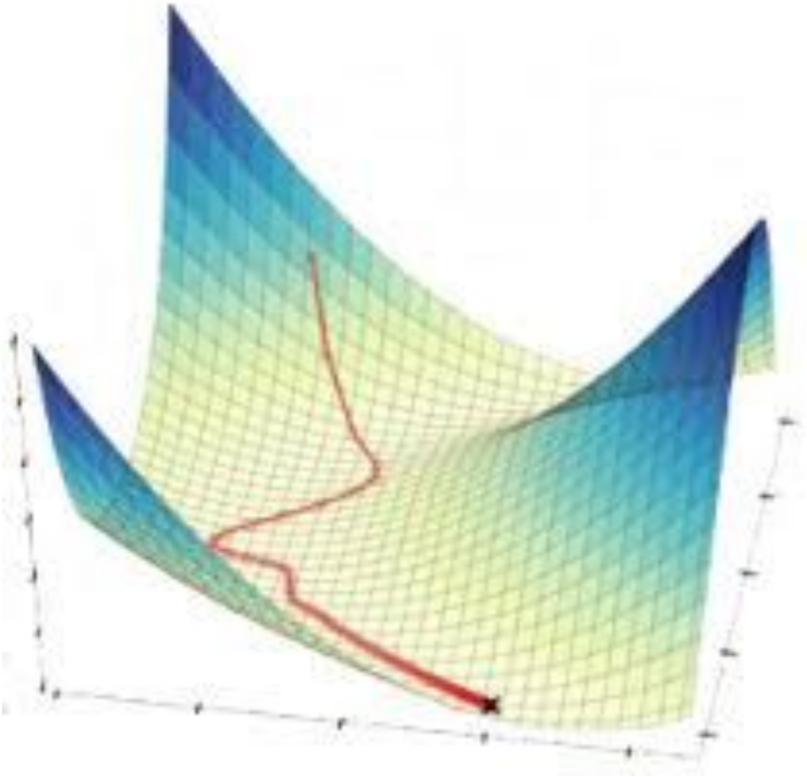
y



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 θ

- 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

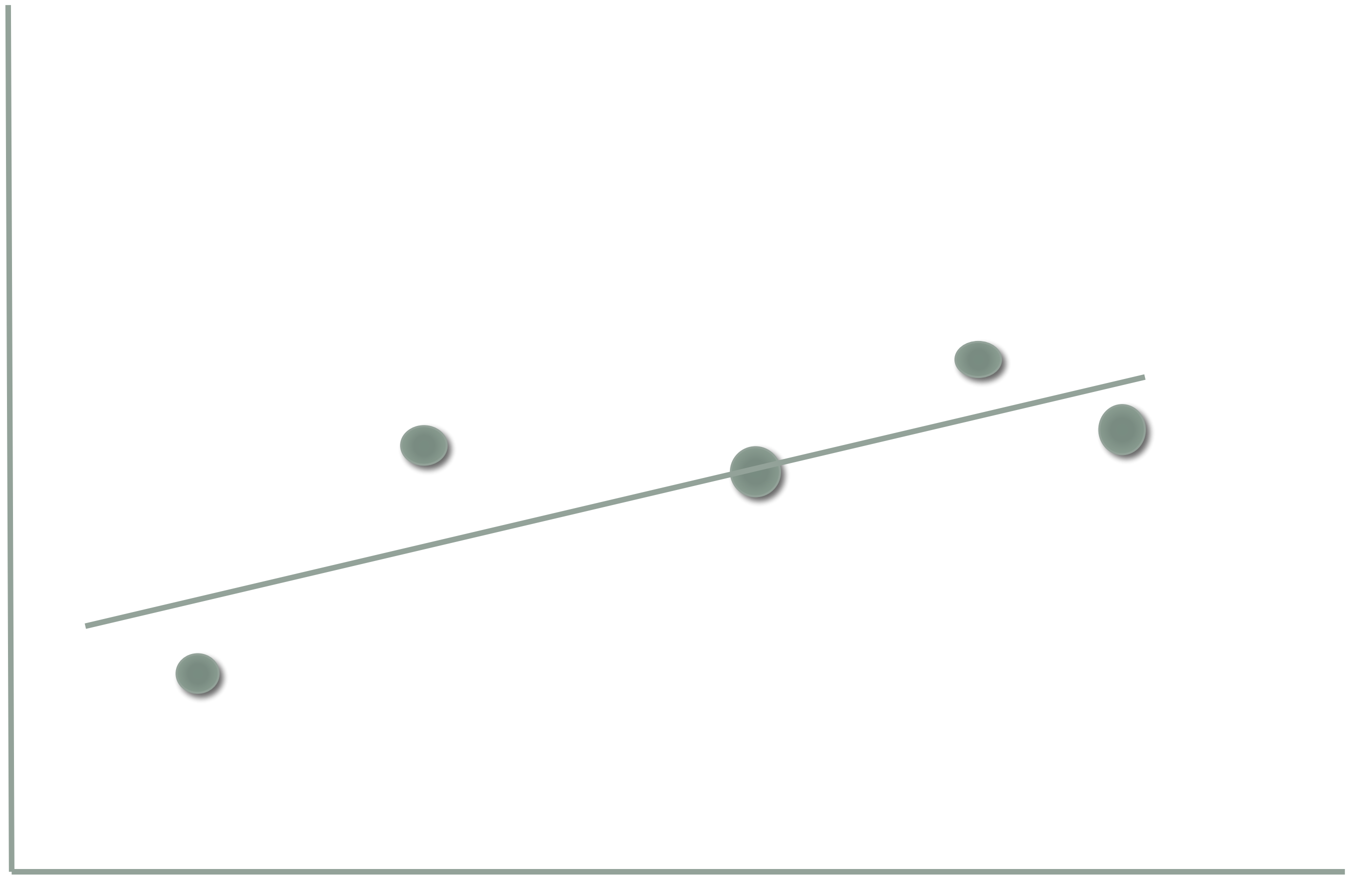
- MSE

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

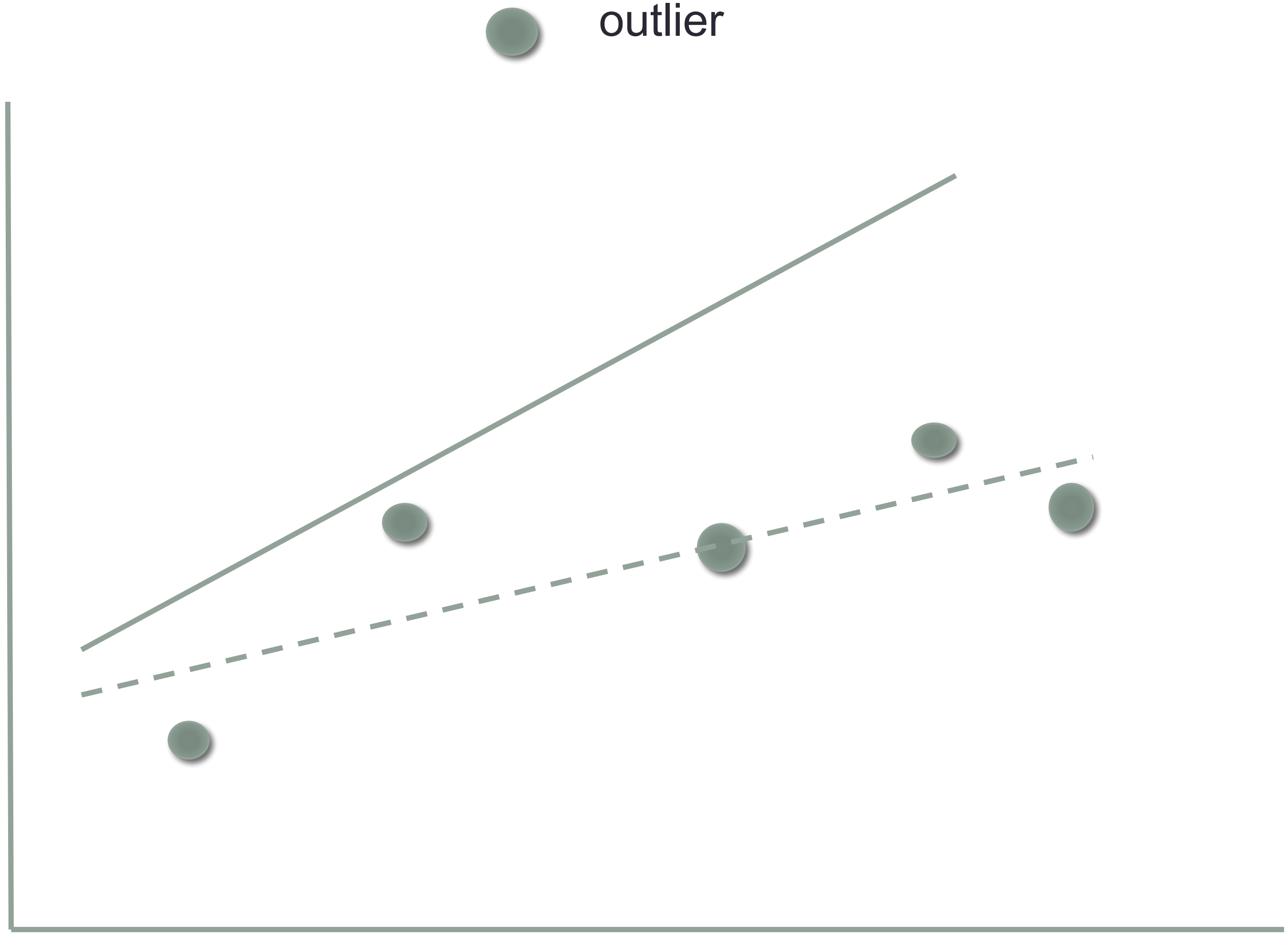
  - Also called L2 loss
- L1 loss

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

L2 vs L1 loss



L2 vs L1 loss



Outlier frequently happens in the real world

Norms (p-norm or Lp-norm)

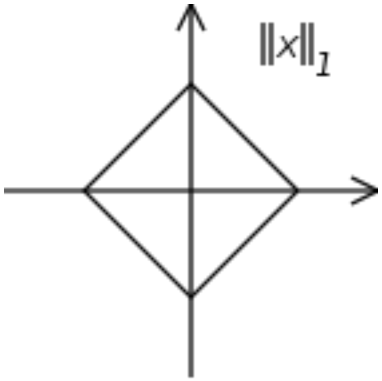
- For any real number p > 1

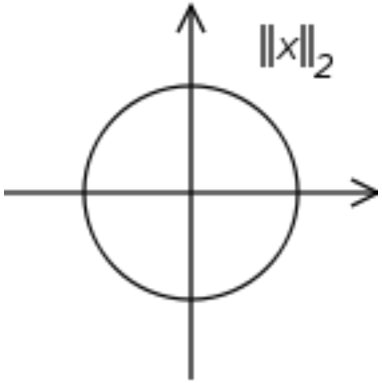
$$||\mathbf{x}||_p = (|x_1|^p + |x_2|^p + ... + |x_n|^p)^{\frac{1}{p}}$$

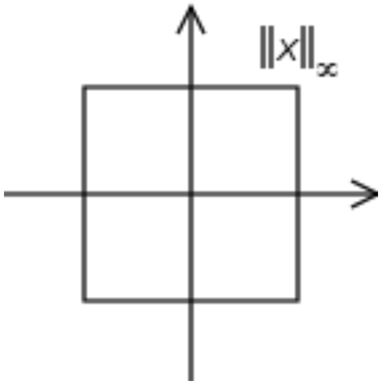
- For p = ∞

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

- 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

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

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

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

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

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

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

$$X\theta - y = \left[\begin{array}{c} x_1^T\theta \\ | \\ x_m^T\theta \end{array}\right] - \left[\begin{array}{c} y_1 \\ | \\ y_m \end{array}\right]$$

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

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 $$\nabla_A trABA^T C = CAB + C^T AB^T$$

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

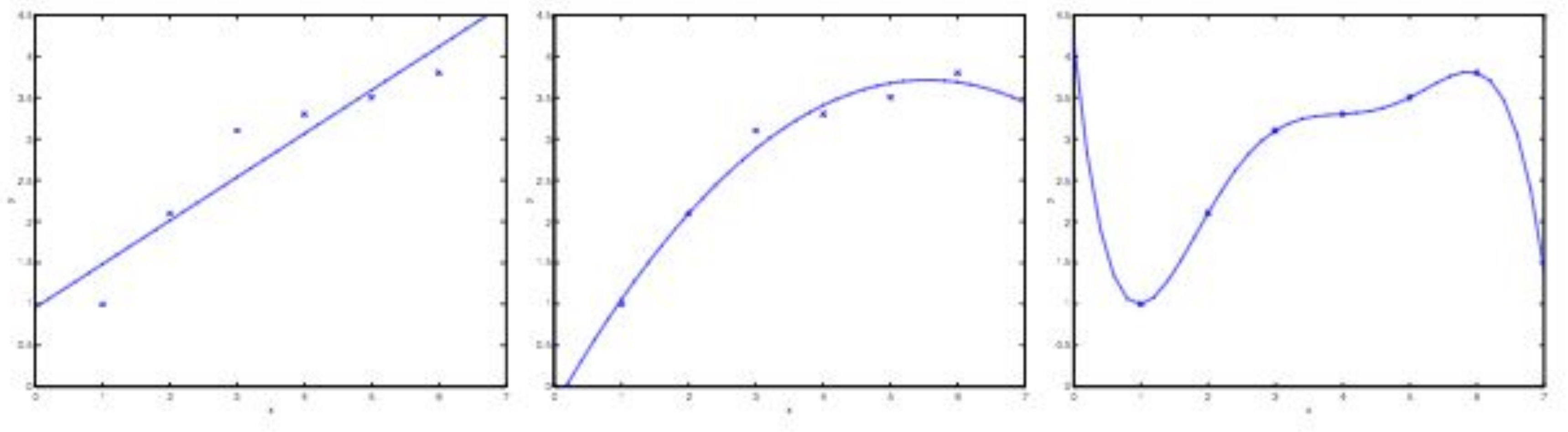
Regression with non-linear features

- 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

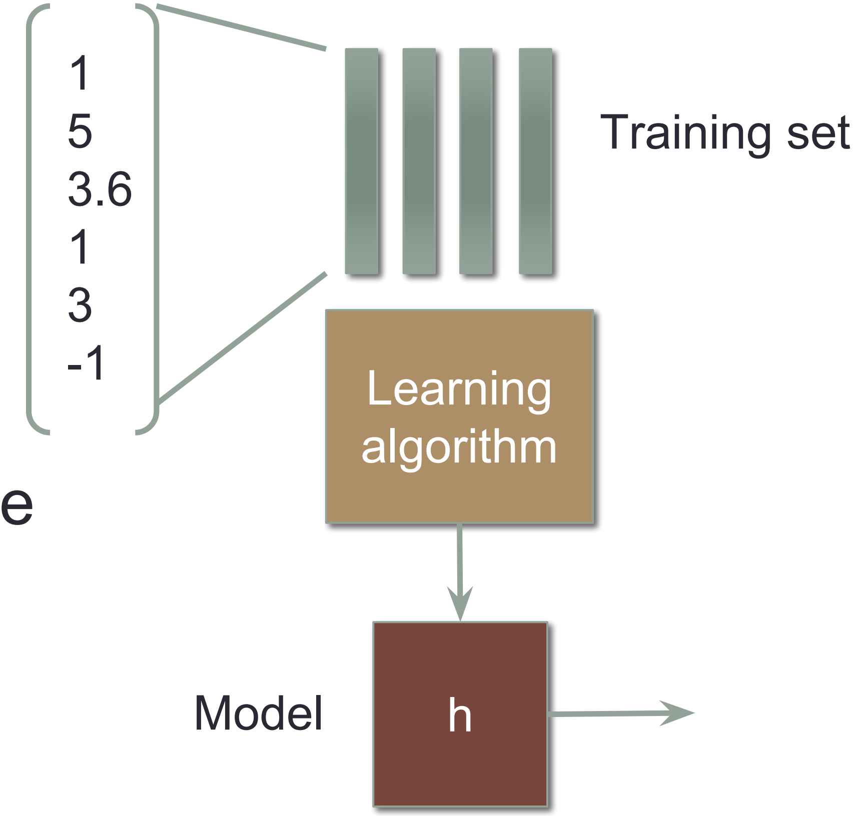
Let’s start with a binary choice. Flood or no flood

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



1
5
3.6
1
3
-1

Training set

Learning algorithm

Model

h

Training phase

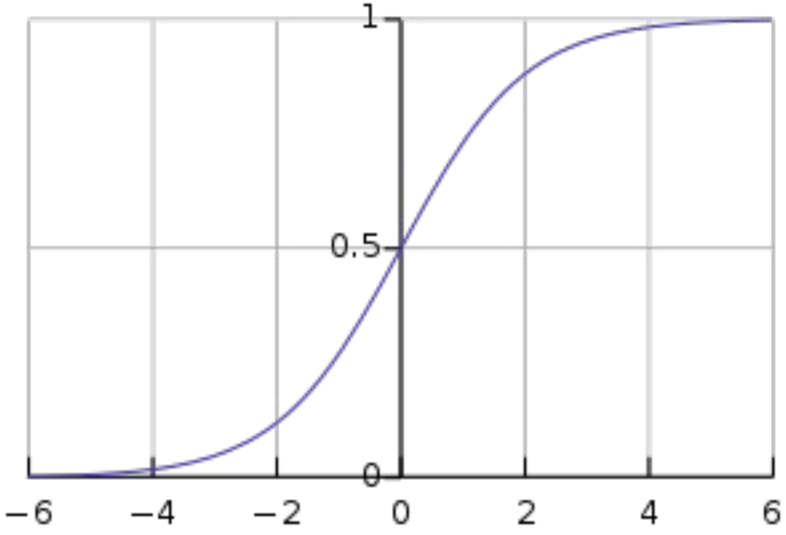
Can we use regression?

- 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

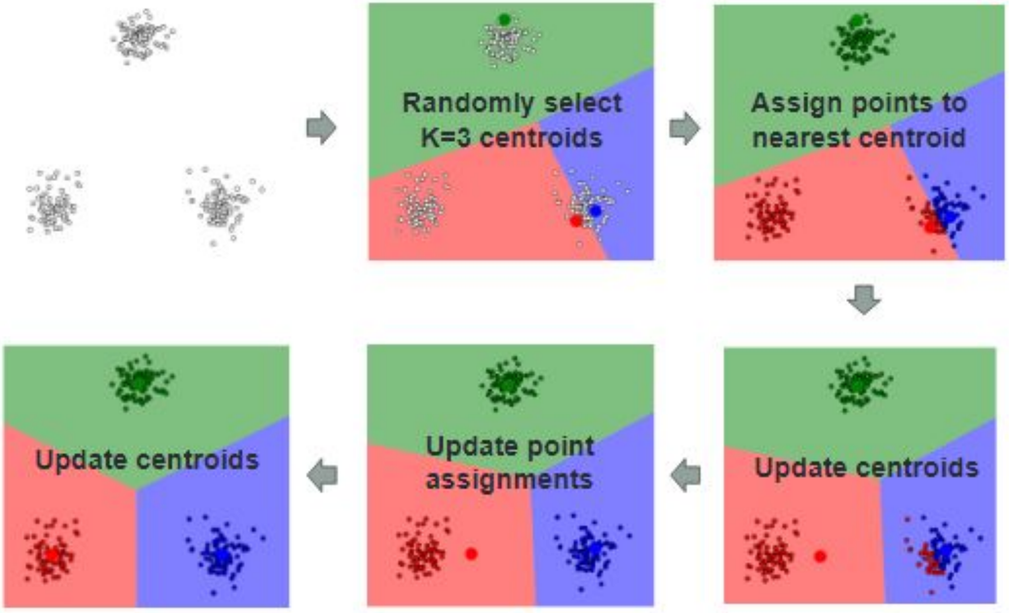
$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

Summary

KNN

K-mean clustering

    Iterative method


Randomly select K=3 centroids
Assign points to nearest centroid
Update centroids
Update point assignments
Update centroids

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)

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

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

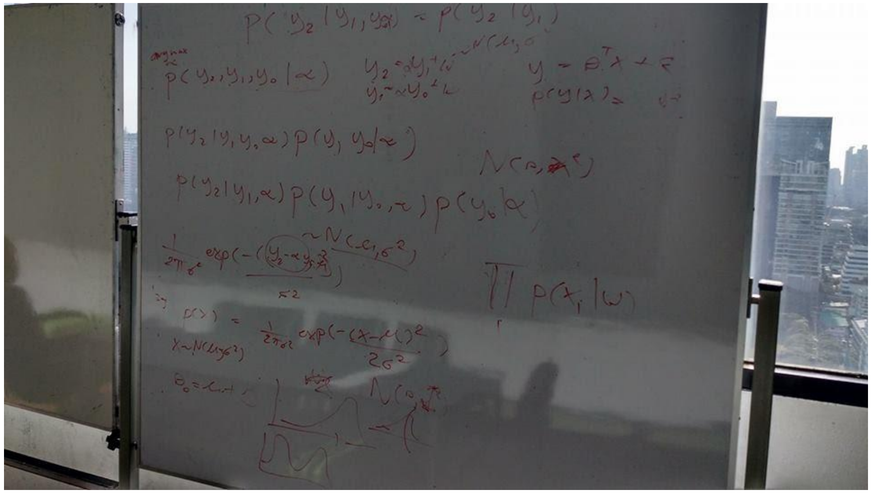
สถิติผลการเสี่ยงทาย "พระโค" กับ ปริมาณฝนเฉลี่ยรายปี
ปี 2550 – 2556
ปี 2550
10,575 มิลลิเมตร
ปี 2551
11,074 มิลลิเมตร
ปี 2552
10,230 มิลลิเมตร
ปี 2553
10,447 มิลลิเมตร
ปี 2554
7,827 มิลลิเมตร
น้ำท่วมใหญ่ !!
ปี 2555
10,959 มิลลิเมตร
ปี 2556
11,428 มิลลิเมตร
ปี 2557
?
ที่มา: กรมอุตุนิยมวิทยา กระทรวงเทคโนโลยีสารสนเทศและการสื่อสาร

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


$p(y_2 | y_1, y_0) = p(y_2 | y_1)$
argmax
$p(y_2, y_1, y_0 | \alpha)$
$y_2 = \alpha y_1 + w \sim N(\mu, \sigma)$
$y_1 \sim \alpha y_0 + w$
$y = \theta^T x + \epsilon$
$p(y|x) =$
$p(y_2 | y_1, y_0, \alpha) p(y_1, y_0 | \alpha)$
$p(y_2 | y_1, \alpha) p(y_1 | y_0, \alpha) p(y_0 | \alpha)$
$\sim N(\mu, \sigma^2)$
$\frac{1}{2\pi\sigma^2} \exp(-\frac{(y_2 - \alpha y_1)^2}{\sigma^2})$
$N(0, \sigma^2)$
$\prod p(x_i | w)$
$p(x) = \frac{1}{2\pi\sigma^2} \exp(-\frac{(x-\mu)^2}{2\sigma^2})$
$x \sim N(\mu, \sigma^2)$
$N(0, \sigma^2)$