

COMP 330/543: Outliers

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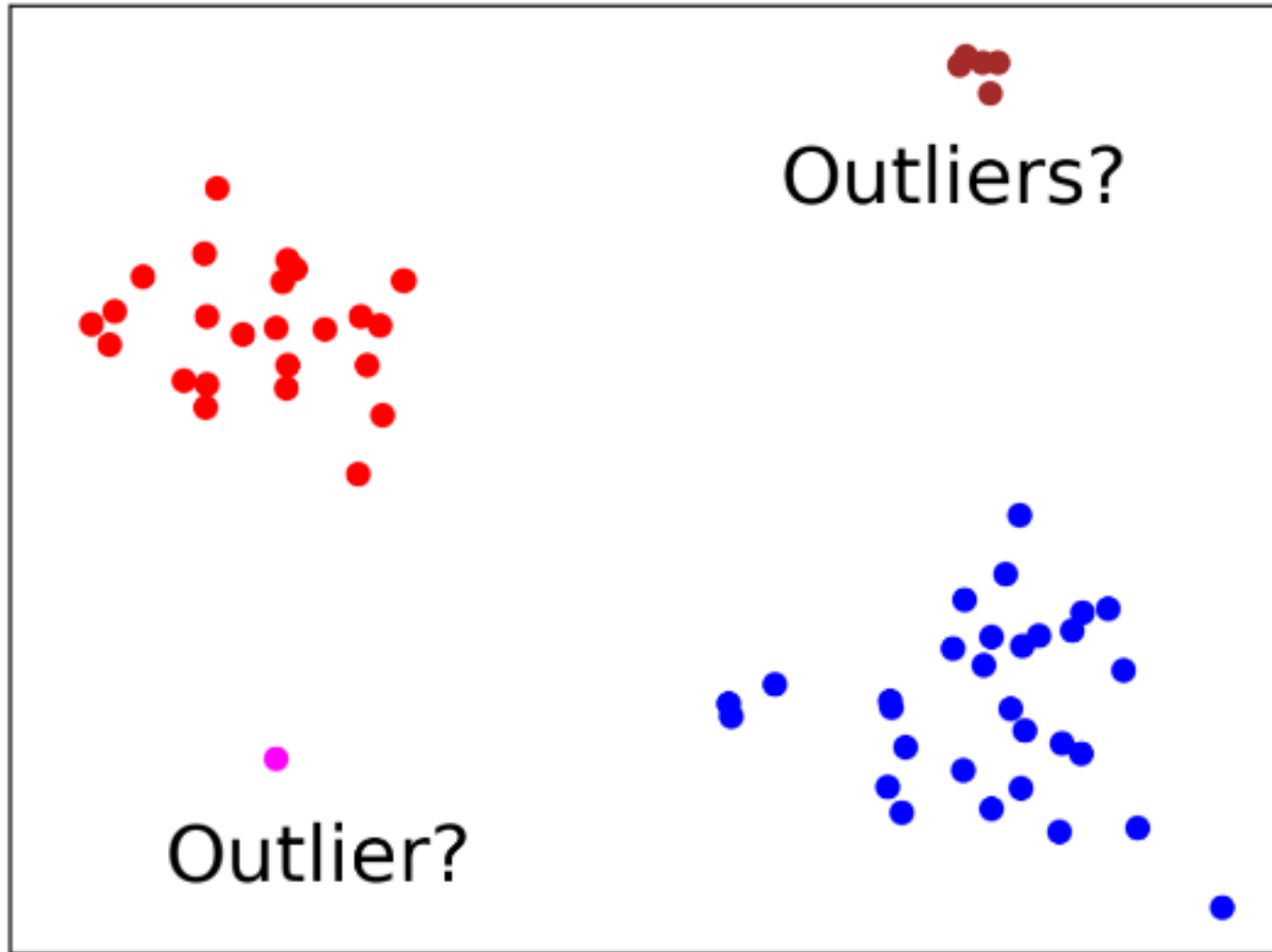
Rice University

What Are Outliers In Data Science?

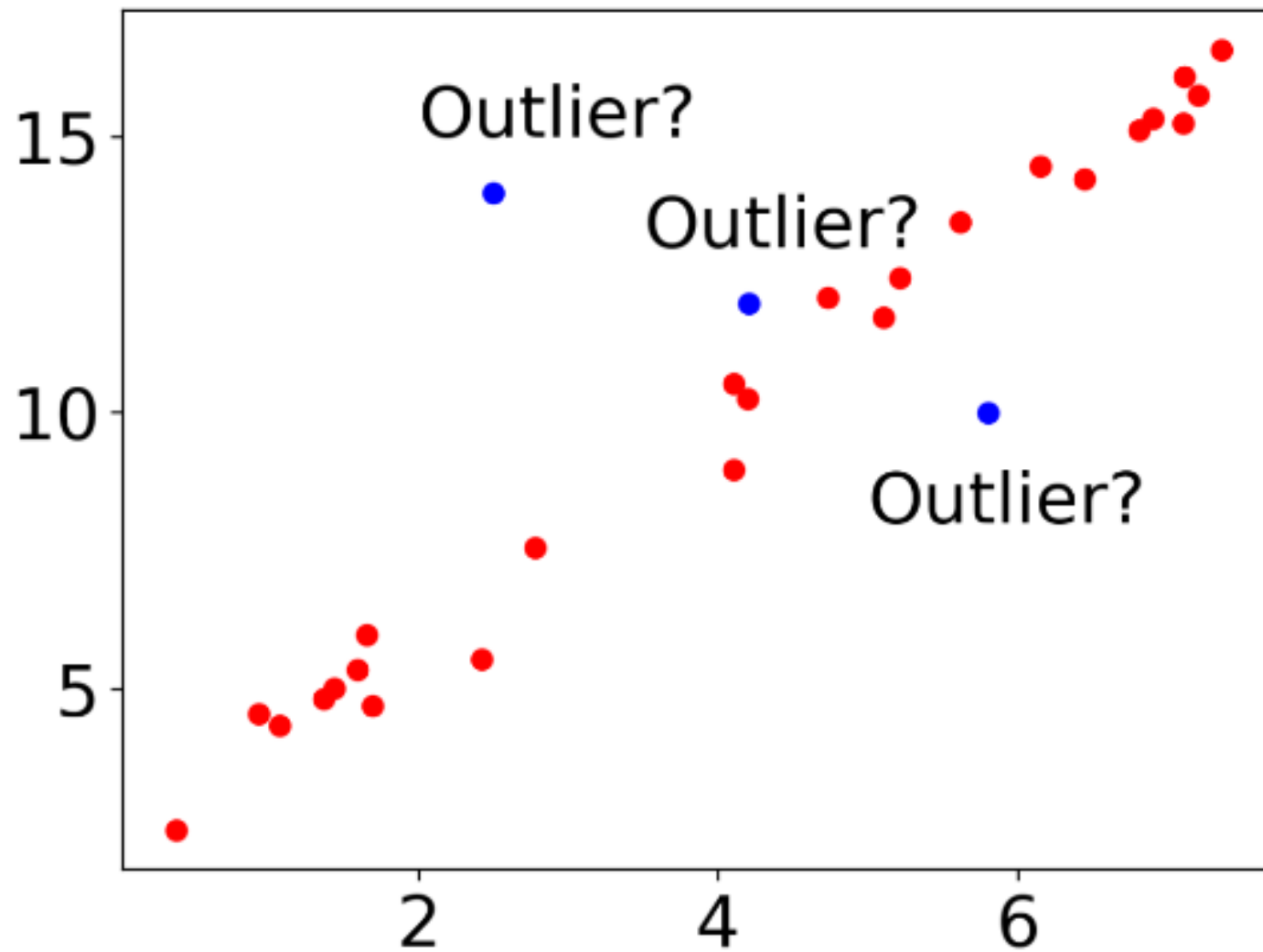
Data points that are unlike the other points, unexpected, or unusual in some way

- Weather data set: low of -12 degrees in Houston
- Sports data set: averaging 10+ rebounds, 10+ assists per game
- Stock trading data set: on day S & P 500 down 300 points, a stock up 10%

Outlier Pic: 1



Outlier Pic: 2



Outliers Not Same As Unusual Data

- Low of 12 degrees in Houston is unusual, probably not an outlier
- Low of -12 in Chicago (a bit) unusual, probably not an outlier
- It's the combination of Houston, -12 that makes this difficult to believe

Why Look For Outliers?

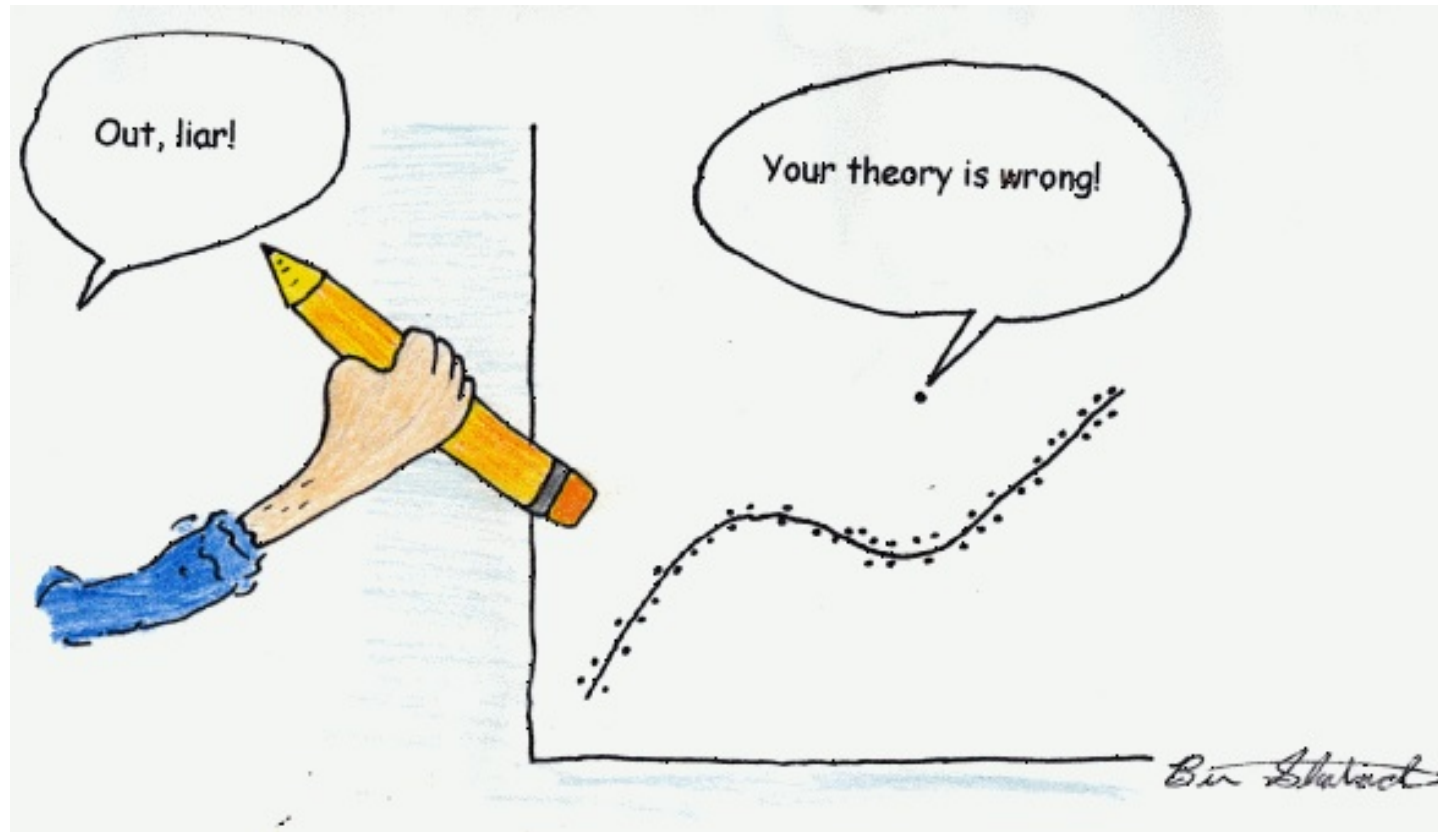
Classically, two reasons:

- To remove them from data...
- ...because outliers can hurt the learning process

Why throw out data?

- It messes up the model
- Garbage in, garbage out
- E.g., huge impact on least squares

But This Can Be Dangerous



Is it really garbage data?

- Values that defy natural laws

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Classically, two reasons:

- (1) Classically, to remove them from data...
- ...because outliers can hurt the learning process
- (2) To find them for further examination...
- ...because outliers might enhance understanding of data

What are some examples where we might want to find outliers?

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What are some examples where we might want to find outliers?

- Computer security
- Fraud detection
- Medical crisis alerts

Outlier Detection is an Unsupervised Task

Why?

Outlier Detection is an Unsupervised Task

Why?

- Supervised learning requires labels
- We don't always know what the outliers look like
- By definition, we don't expect them
- They are rare and unexpected

How Do We Define Outliers?

Two standard definitions:

- (1) Distance-based
- (2) Model-based

Distance-Based Outliers

Def: A point is an outlier if it is far from all other points

Outlier search often defined in terms of k NN:

- Let $d(x_i)$ be the distance to point x_i 's k th NN in the data set
- Then given data set $\langle x_1, x_2, \dots, \rangle$, we want to compute the set O such that...
- $|O| = m$ and $\forall (x_o \in O, x_i \in X - O), d(x_i) \leq d(x_o)$

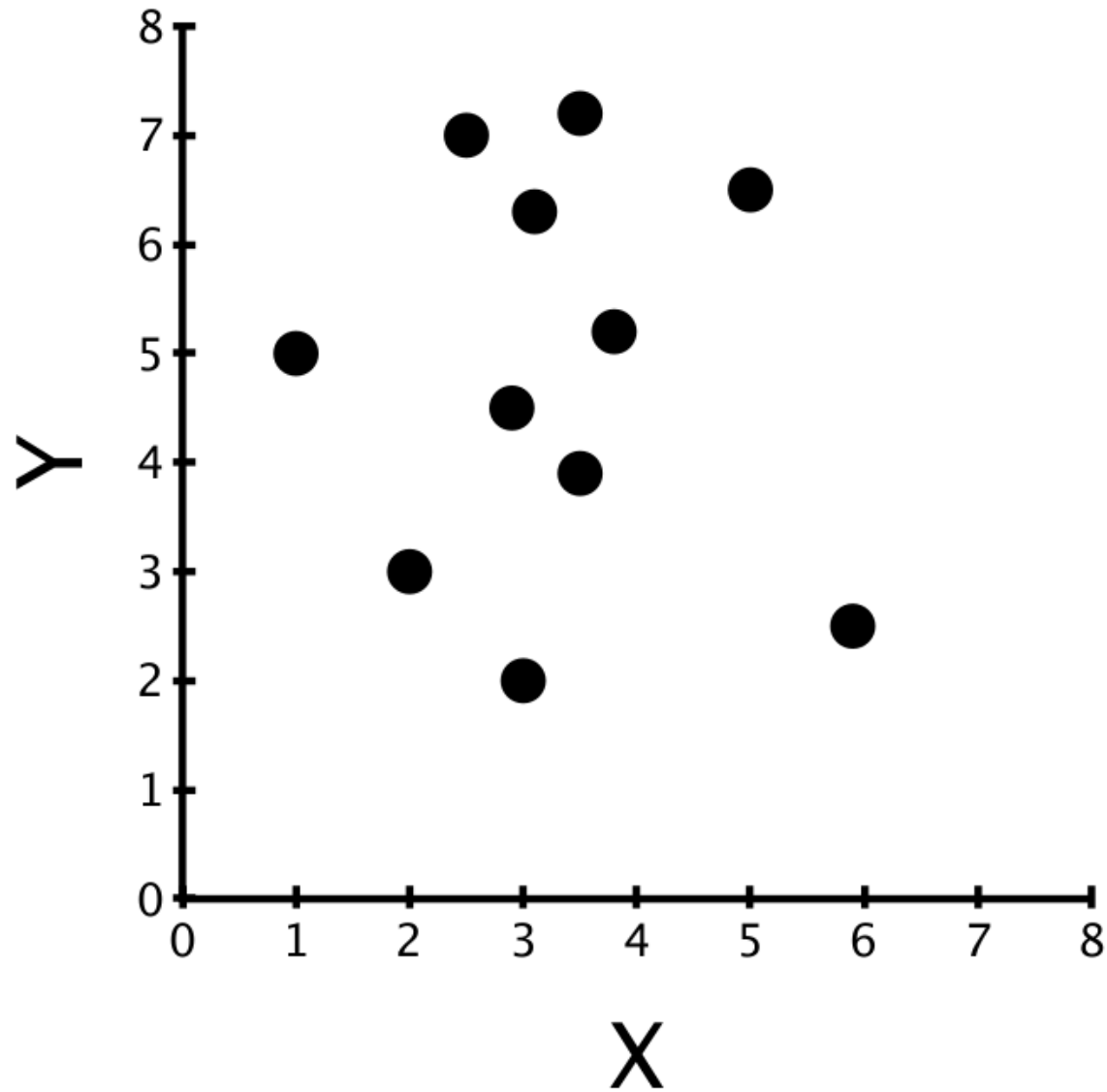
How To Find Distance-Based Outliers?

Simple algorithm:

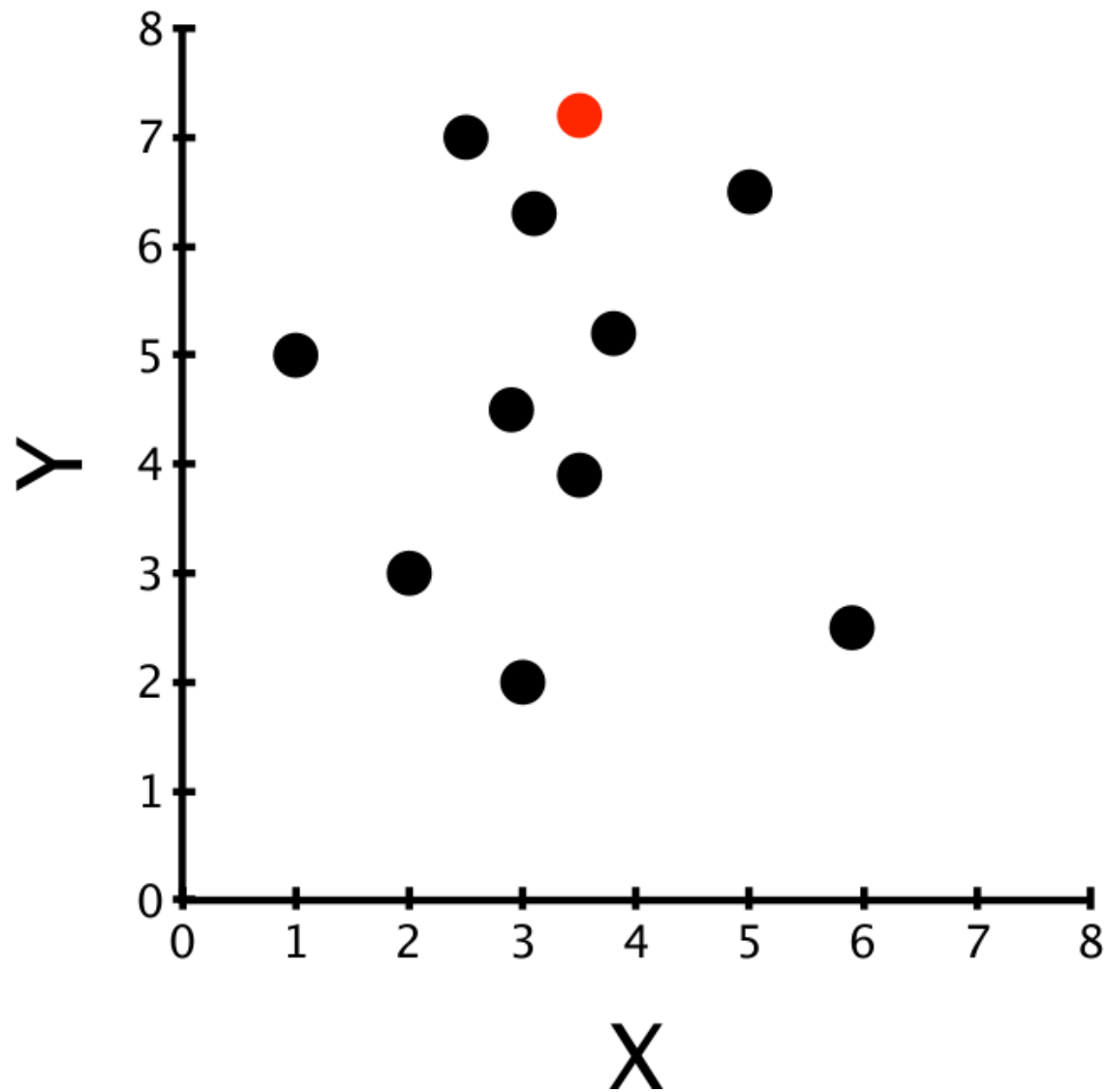
```
init min-priority queue  $O$ 
for  $x_1 \in X$ :
    init max-priority queue  $P$ 
    for  $x_2 \neq x_1 \in X$ :
        insert  $\text{dist}(x_1, x_2)$  into  $P$ 
        if  $|P| > k$ 
            remove max from  $P$ 
    insert  $x_1$  into  $O$  with key  $\text{max}(P)$ 
    if  $|O| > m$ 
        remove point with min key from  $O$ 

return  $O$ 
```

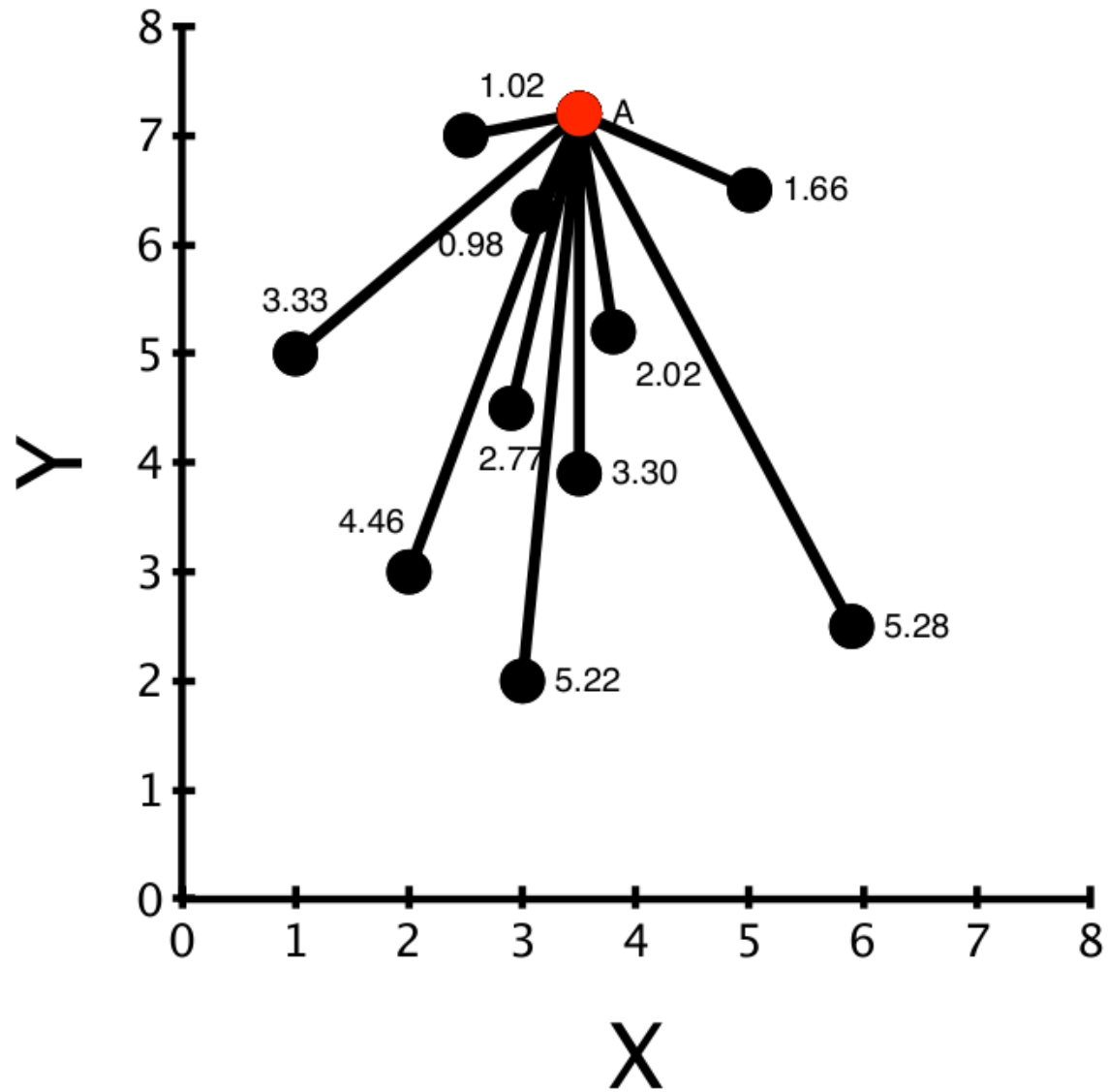
Example: 2NN



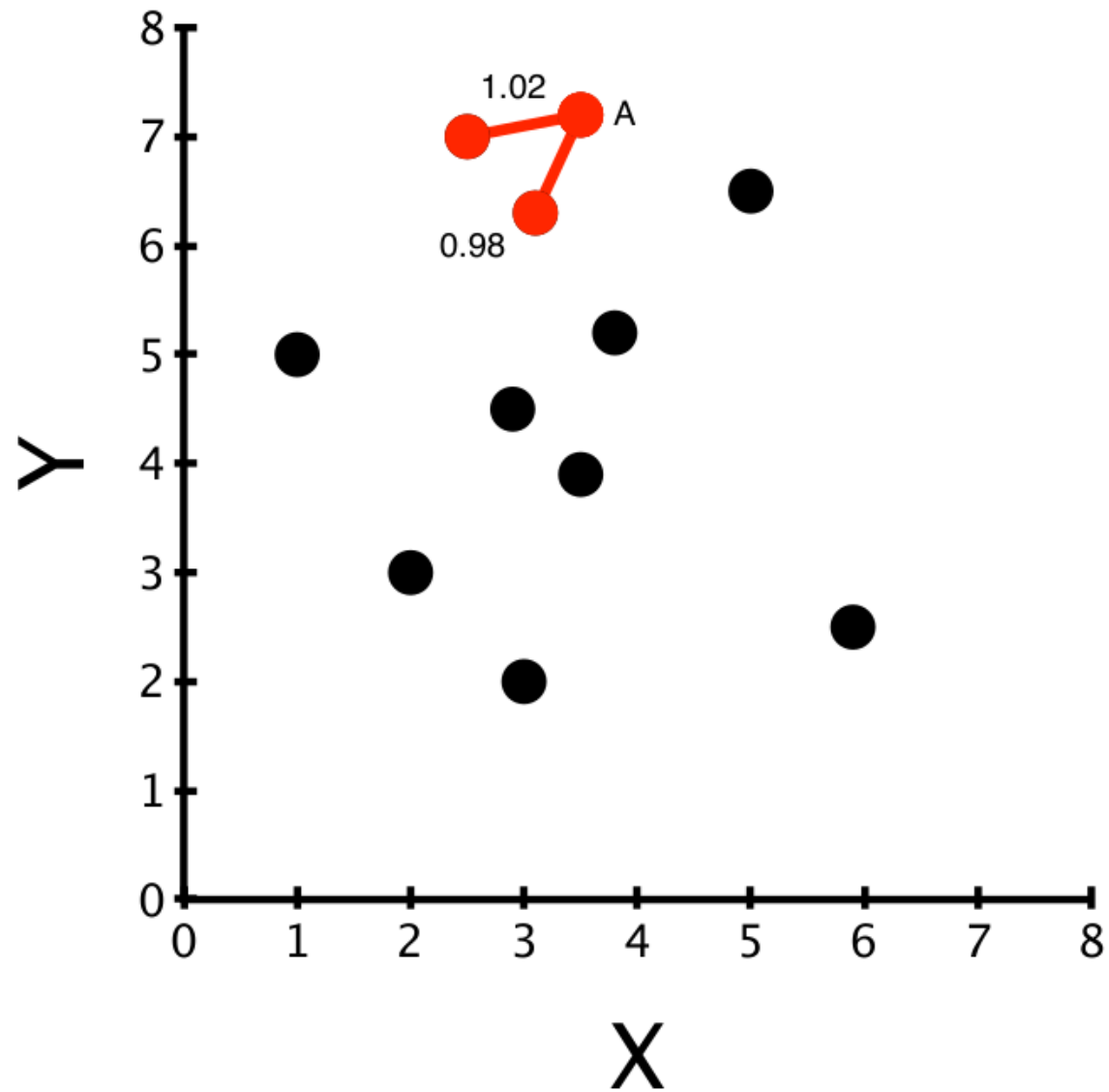
Example: 2NN



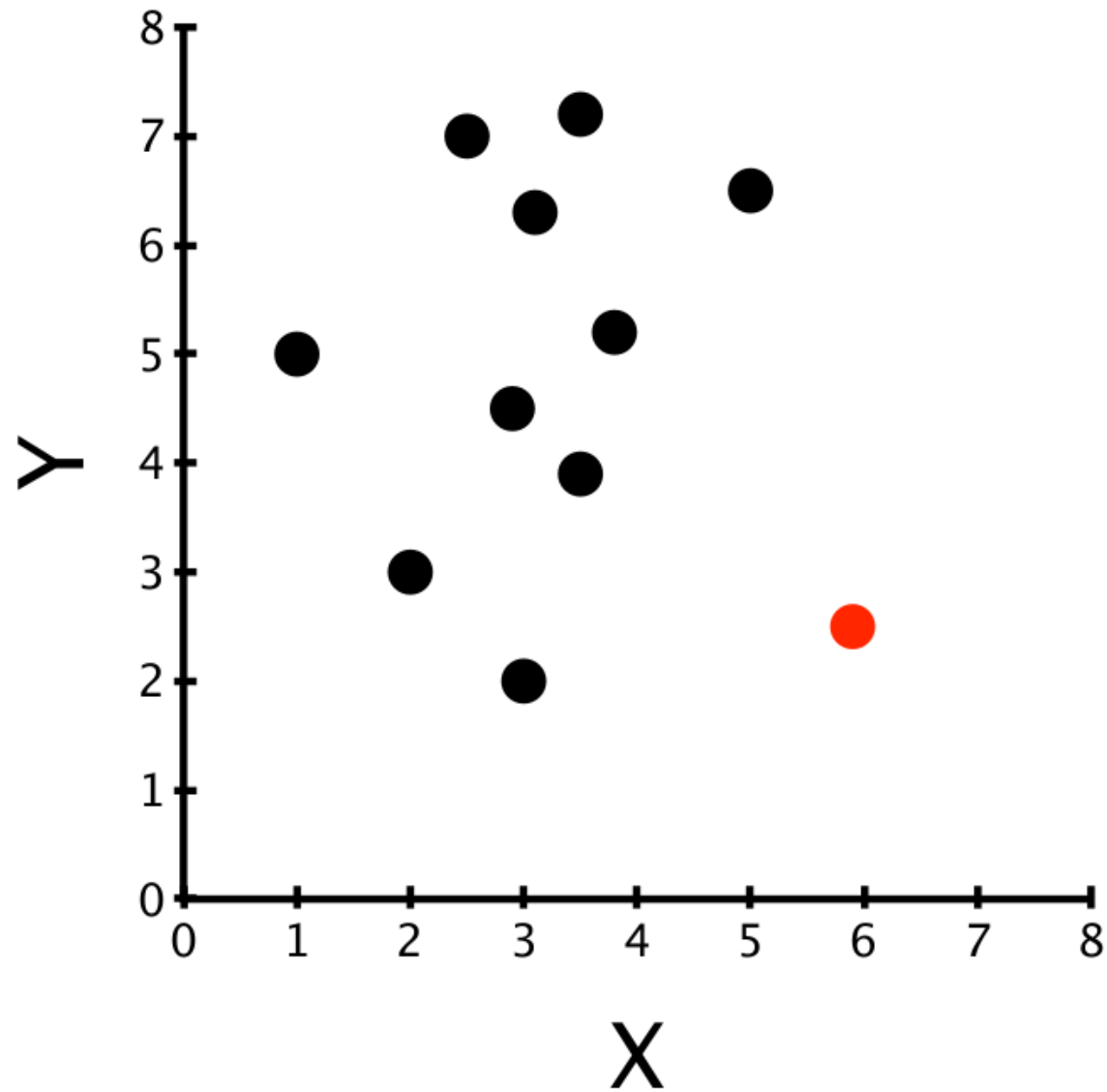
Example: 2NN



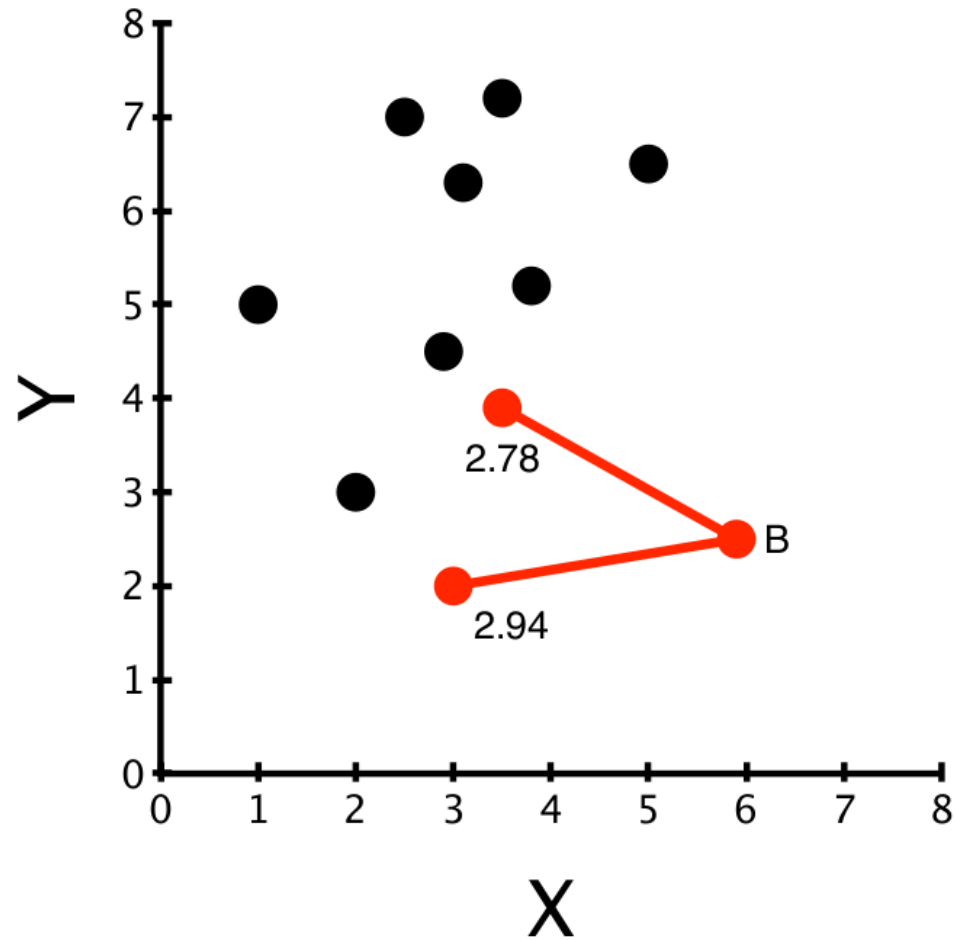
Example: 2NN



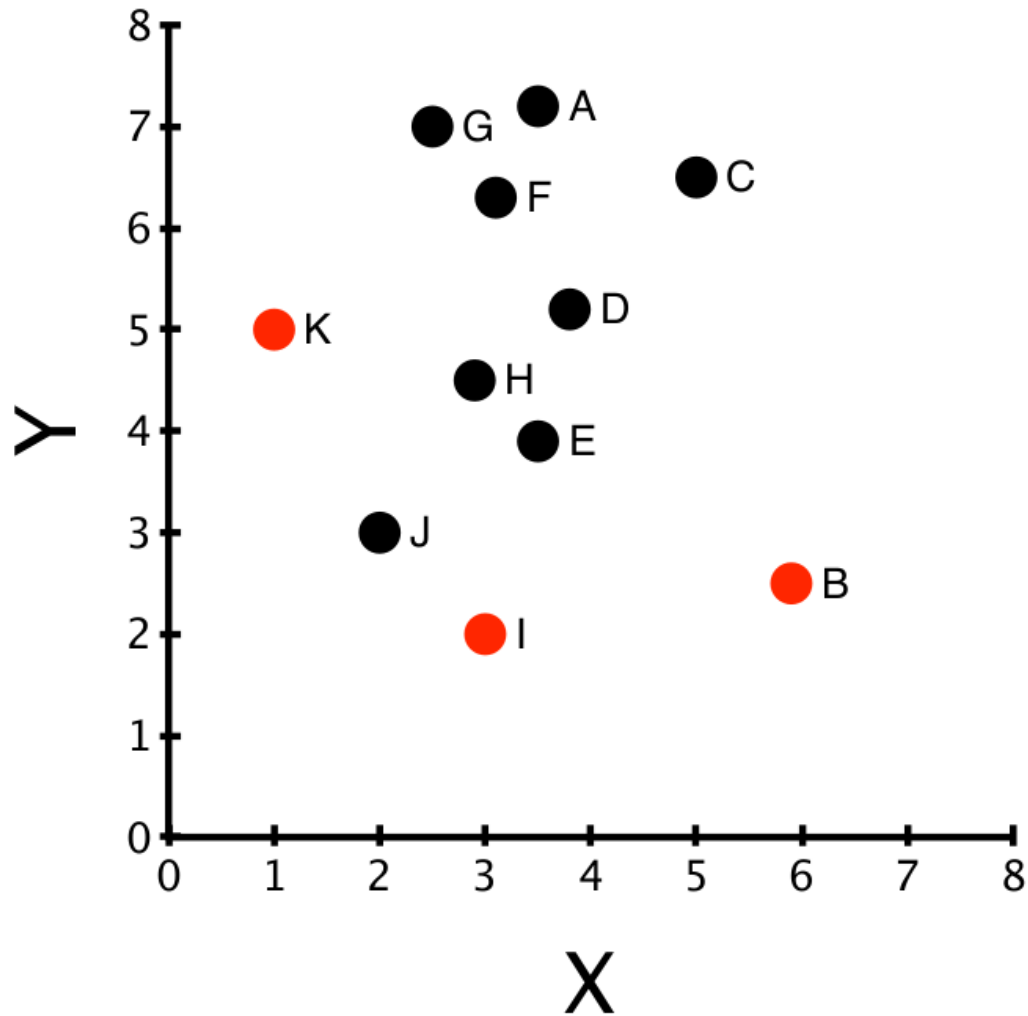
Example: 2NN



Example: 2NN



Example: 2NN $m = 3$



| Point | 2NN distance |
|-------|--------------|
| A | 1.02 |
| B | 2.94 |
| C | 1.77 |
| D | 1.30 |
| E | 1.33 |
| F | 0.98 |
| G | 1.02 |
| H | 1.14 |
| I | 1.96 |
| J | 1.75 |
| K | 2.24 |

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return  $O$ 
```

- So the algorithm works... What's the problem here?

How To Find Distance-Based Outliers?

What's the problem here?

- Nested loop through the entire database
- Too slow for big data
- How to address?

How To Find Distance-Based Outliers?

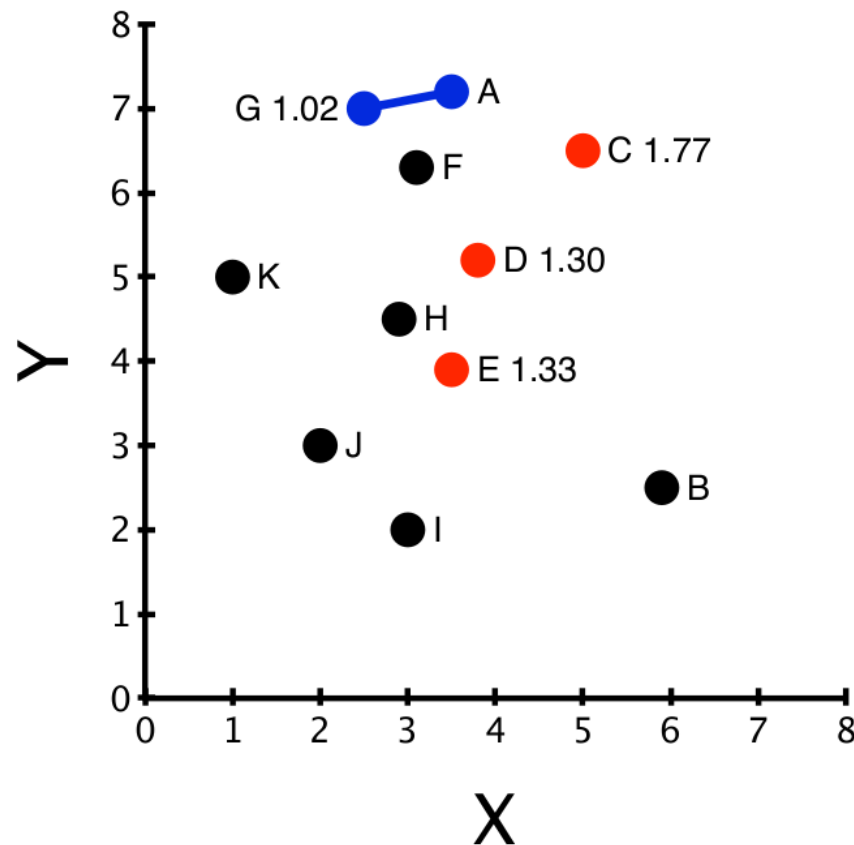
Better algorithm:

```
init min-priority queue  $O$ 
for  $x_1 \in X$ :
    init max-priority queue  $P$ 
    for  $x_2 \neq x_1 \in X$ :
        insert  $\text{dist}(x_1, x_2)$  into  $P$ 
        if  $|P| > k$ 
            remove max from  $P$ 
        if  $|P| == k$  and  $|O| == m$  and  $\text{max}(P) < \text{min}(O)$ 
            discard  $x_1$ ; not an outlier
    insert  $x_1$  into  $O$  with key  $\text{max}(P)$ 
    if  $|O| > m$ 
        remove point with min key from  $O$ 

return  $O$ 
```


How To Find Distance-Based Outliers?

- Example: O: $\{(1.33, E), (1.77, C), (1.3, D)\}$
- Process A, find 2-NN where $dist(A, F) = 0.98$, discard A



How To Find Distance-Based Outliers?

Why does this help?

- $\max(P)$ is an upper bound on distance to k th NN
- So distance to k th NN can't ever be greater
- If this is not good enough to get point into top m in O
- Then can discard it early
- Can get a 100x speed up
- Still $O(N^2)$

How To Find Distance-Based Outliers?

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Even better:

- Store X in randomized order
- Lower chances of getting unlucky and finding all far points first

What About the hyper-parameters

How to compute $\text{dist}(x, y)$?

- Classical method: if x, y vectors, use l_p norm of $x - y$

How to choose m ?

- Very application specific
- Start small, gradually increase it
- Stop when nothing "interesting" is added

How to choose k ?

- Empirically determined using the validation set
- Try \sqrt{N}

Model-Based Outliers

Basic idea:

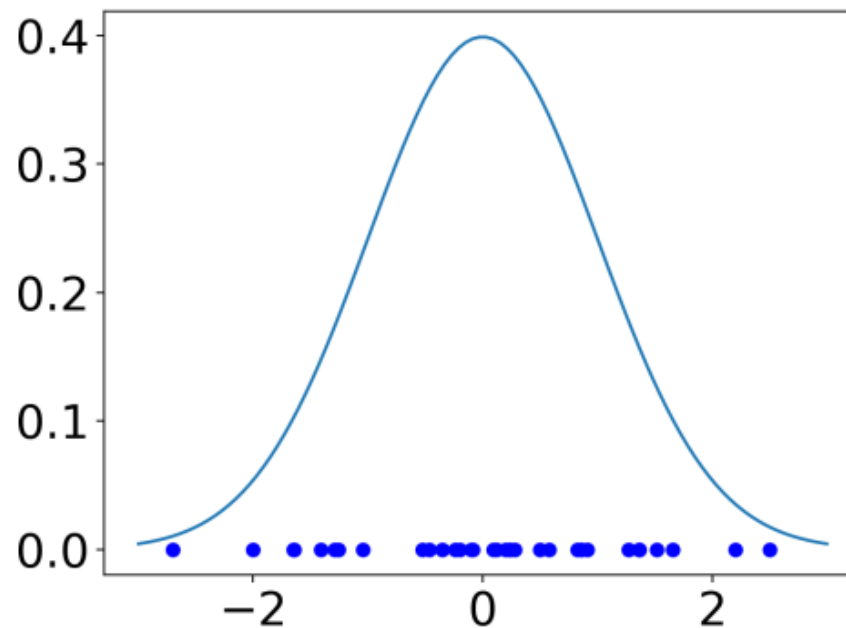
- Learn a model for what is “typical”
- Might be probabilistic
- Might be least-squares
- Then outlier is a data point with a low score according to the model

Example of Model-Based Detection

Learn Normal distribution by choosing $\{\mu\}, \{\sigma^2\}$ to maximize

$$P(x_1, x_2, \dots, x_n) = \prod_i \text{Normal}(x_i | \mu, \sigma^2)$$

Then choose m points with smallest $\text{Normal}(x_i | \mu, \sigma^2)$



Questions?