Master's degree ICT Internet Multimedia Engineering

DENSITY BASED CLUSTERING: DBSCAN

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DIPARTIMENTO DI INGEGNERIA DELL'INFORMAZIONE

DIPARTIMENTO MATEMATICA

UNIVERSITÀ DEGLI STUDI DI PADOVA

Overview

- Reference papers
- Partition *vs* density-based clustering
- DBSCAN
  - Rationale, main features
  - Density reachability
  - Density connected points
- DBSCAN algorithm
- Examples, discussion
- Setting DBSCAN pars?

Reference papers

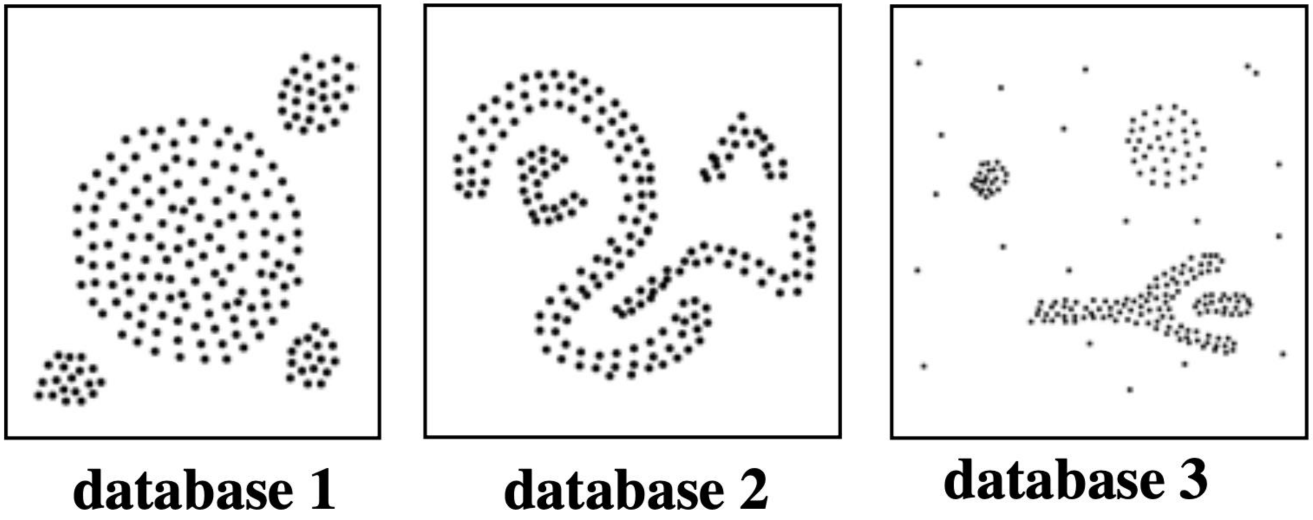
[Ester96] Martin Ester, Hans-Peter Kriegel, Joerg Sander, Xiaowei Xu, A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise, 2nd International Conference on Knowledge Discovery and Data Mining (KDD), 1996. [33856 citations, Oct 2024]

[Shubert] Eric Shubert, Joerg Sander, Martin Ester, Hans Peter Kriegel, Xiaowei Xu, DBSCAN Revisited, Revisited: Why and How You Should (Still) Use DBSCAN, ACM Transactions on Database Systems, No. 19, July 2017. [2583 citations, Oct 2024]

Partition *vs* density-based clustering

- Partitioning algorithms (e.g., K-means and the like)
  - N objects, to cluster into K classes
  - K is known
- Usual two-step procedure
  - Determine K by minimizing an objective (cost) function
  - Assign each object to the closest cluster: this means that a partition is equivalent to a Voronoi diagram → each cluster is contained in a Voronoi cell → clusters tend to be convex
- Problem
  - Convex clusters are not always appropriate

Density based notion of clusters



- We, as humans, easily recognize the clusters
- Main reasons
  - Density of points is considerably *higher* than outside the clusters
  - Density within the areas of noise is *lower* than that of any cluster

DBSCAN: pars & Eps-neighborhood

- Uses 2 parameters: (Eps, MinPts)
- Eps: radius of the neighborhood
- MinPts: min. no. of points in an Eps-neighborhood
- Eps-Neighborhood of point p

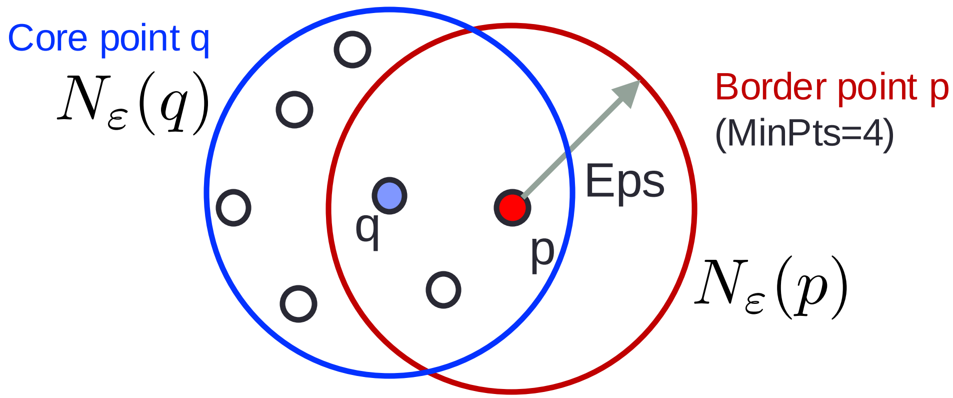
$$N_\varepsilon(p) = \{q \in \mathrm{dataset} \mid \mathrm{dist}(p, q) \leq \epsilon\}$$

- Remarks
  - Any distance function can be used
  - Points p,q can be vectors in a space of any number of dimensions

DBSCAN: review of features

- Single scan of data points
- Clustering based on density (local criterion)
  - Region around a point: within a distance Eps (any distance metric)
  - Density of a region: more than MinPts within a region
  - Core point
    - whose “Eps-neighborhood” contains at least MinPts points
  - Border point
    - fewer than MinPts within Eps-neighborhood
    - but density reachable from a core point
  - Two points belong to the same cluster
    - if connected by a dense region of points (see later)
- DBSCAN handles noise
  - Points that are not enrolled in any valid cluster → treated as noise

Def. directly density reachabile

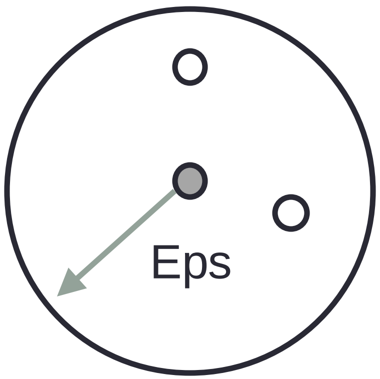


- p is directly density reachable from q wrt (Eps, MinPts) IF
  1. p is within Eps-neighborhood of q, $N_\varepsilon(q)$
  2. q is a core point, i.e., $|N_\varepsilon(q)| \geq \mathrm{MinPts}$

NOTE: this relationship is ***asymmetric***

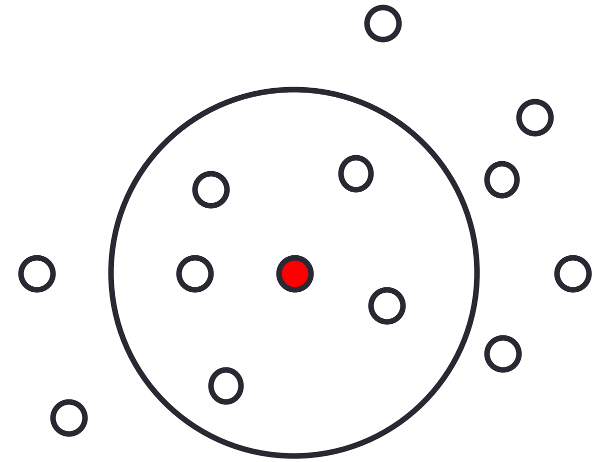
- in the above figure, q is not density reachable from p, as p is not a core point (does not meet the local density criterion)

Summary of point types



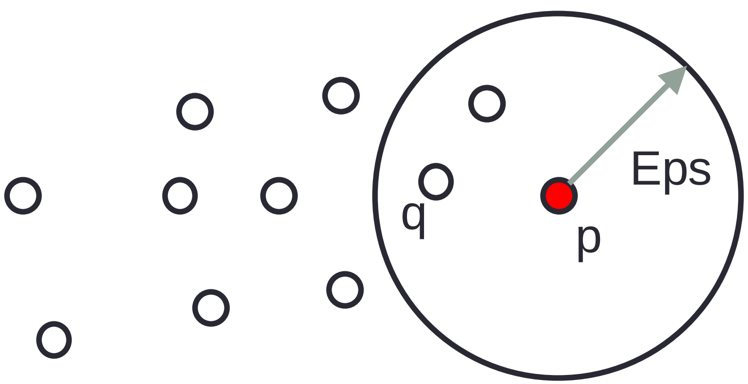
Noise point (MinPts=4)

1. has fewer than MinPts within Eps
2. no neighbor is a core point



Core point (MinPts=4)

1. has more than MinPts within Eps



Border point p (MinPts=4)

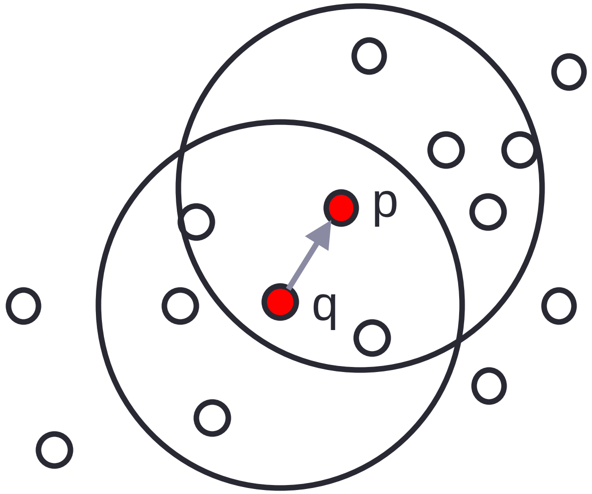
1. has fewer than MinPts within Eps
2. at least one core point (e.g., q) within Eps

Density reachability example (direct)

MinPts=4

- The two red points are within reach and density connected
- They are both core points as
  - they have more than MinPts within their Eps-beighborhood
- p is density reachable from q and vice versa
- In this case the relation holds in both ways (p→q, q→p)

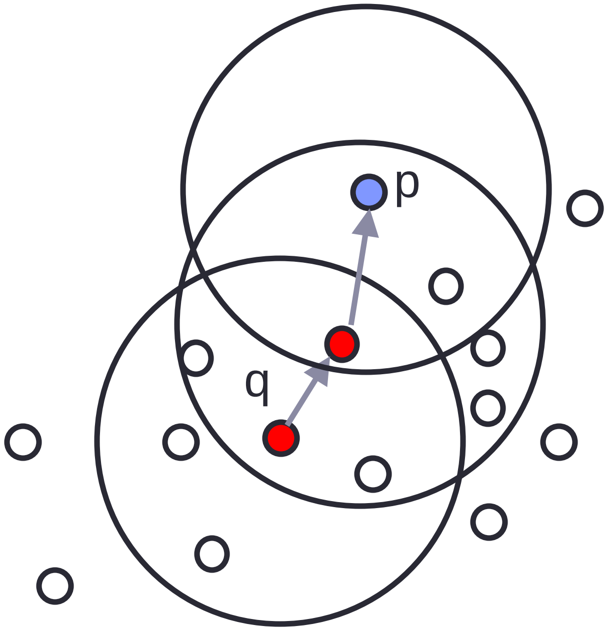
→ not true in general



Density reachability example (path)

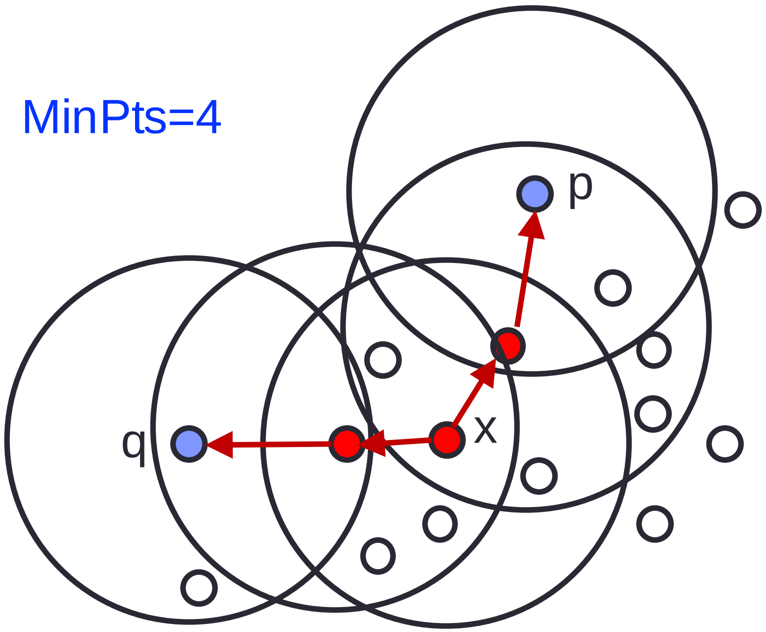
MinPts=4

- point p is density reachable from point q (via a multi-hop relationship)
- q is not density reachable from p, as p in this case is not a core point
- density reachability is in general asymmetric



Density connected points

- Any two points are density connected: if there exists another point x such that they are both density reachable from x
- Example in the figure: p and q are border points
  - are density connected to each other by point x
  - the red points are all core points



DBSCAN: main loop

- SetOfPoints: all the points in the dataset
- Eps, MinPts: DBSCAN parameters

```
DBSCAN (SetOfPoints, Eps, MinPts)

// SetOfPoints is UNCLASSIFIED
  ClusterId := nextId(NOISE);
  FOR i FROM 1 TO SetOfPoints.size DO
    Point := SetOfPoints.get(i);
    IF Point.ClId = UNCLASSIFIED THEN
      IF ExpandCluster(SetOfPoints, Point,
                ClusterId, Eps, MinPts) THEN
        ClusterId := nextId(ClusterId)
      END IF
    END IF
  END FOR
END; // DBSCAN
```

Try to expand a cluster of density connected points from each point in the dataset

Once the cluster has been computed for a point i, switch to the next point, advancing the Cluster ID counter

If a point was already assigned a ClusterID (included in a cluster) in a previous expand action → skip it

DBSCAN: ExpandCluster

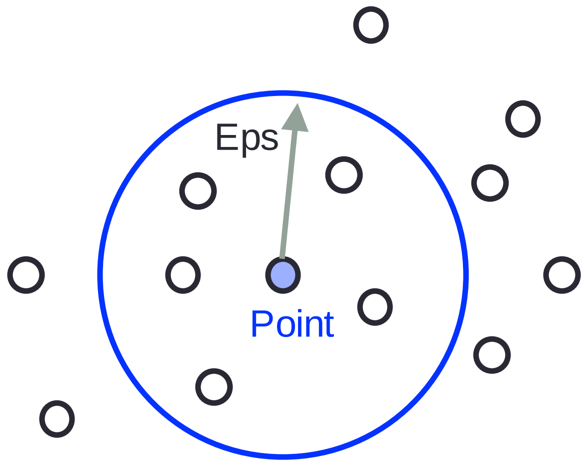
```
ExpandCluster(SetOfPoints, Point, ClId, Eps,
              MinPts) : Boolean;
  seeds:=SetOfPoints.regionQuery(Point,Eps);
  IF seeds.size<MinPts THEN // no core point
    SetOfPoint.changeClId(Point,NOISE);
    RETURN False;
  ELSE   // all points in seeds are density-
         // reachable from Point
    SetOfPoints.changeClIds(seeds,ClId);
    seeds.delete(Point);
    WHILE seeds <> Empty DO
      currentP := seeds.first();
      result := SetOfPoints.regionQuery(currentP,
                                         Eps);
      IF result.size >= MinPts THEN
        FOR i FROM 1 TO result.size DO
          resultP := result.get(i);
          IF resultP.ClId
              IN {UNCLASSIFIED, NOISE} THEN
            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```

It starts with:

- point Point, which is UNCLASSIFIED

seeds = SetOfPoints.regionQuery()

- seeds: a set cointaining all the points that are within distance Eps (the so called "Eps-neighborhood" of Point)



seeds → Eps-neighborhood
MinPts=4

DBSCAN: ExpandCluster

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ExpandCluster(SetOfPoints, Point, ClId, Eps,
               MinPts) : Boolean;
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  ELSE    // all points in seeds are density-
          // reachable from Point
    SetOfPoints.changeClIds(seeds,ClId);
    seeds.delete(Point);
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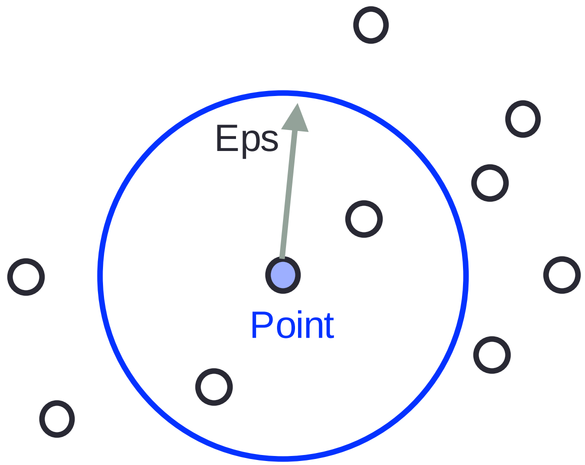
                                           Eps);
      IF result.size >= MinPts THEN
        FOR i FROM 1 TO result.size DO
          resultP := result.get(i);
          IF resultP.ClId
              IN {UNCLASSIFIED, NOISE} THEN
            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```

If seeds contains fewer than MinPts → Point is marked as NOISE

Point cannot be a core point

NOTE: the NOISE label can be changed at a later stage, if Point is density reachable from some other (core) point in the dataset



Point → NOISE
MinPts=4

DBSCAN: ExpandCluster

```
ExpandCluster(SetOfPoints, Point, ClId, Eps,
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                                          Eps);
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              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```

all the points in seeds are density-reachable from Point (by construction)

hence, all these points take the same cluster ID (ClId) of Point

→ SetOfPoints.changeClIds(seeds,ClId)

DBSCAN: ExpandCluster

```
ExpandCluster(SetOfPoints, Point, ClId, Eps,
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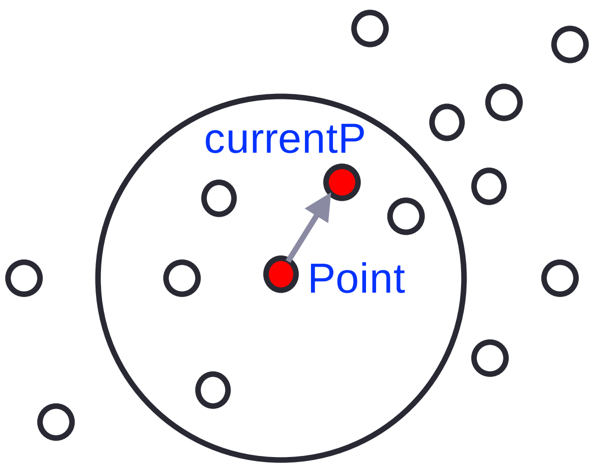
              IN {UNCLASSIFIED, NOISE} THEN
            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```

remove Point from the seeds set

scan all the remaining points in the seeds set → currentP is the first of such points



DBSCAN: ExpandCluster

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    seeds.delete(Point);
    WHILE seeds <> Empty DO
      currentP := seeds.first();
      result := SetOfPoints.regionQuery(currentP,
                                        Eps);
      IF result.size >= MinPts THEN
        FOR i FROM 1 TO result.size DO
          resultP := result.get(i);
          IF resultP.ClId
              IN {UNCLASSIFIED, NOISE} THEN
            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```
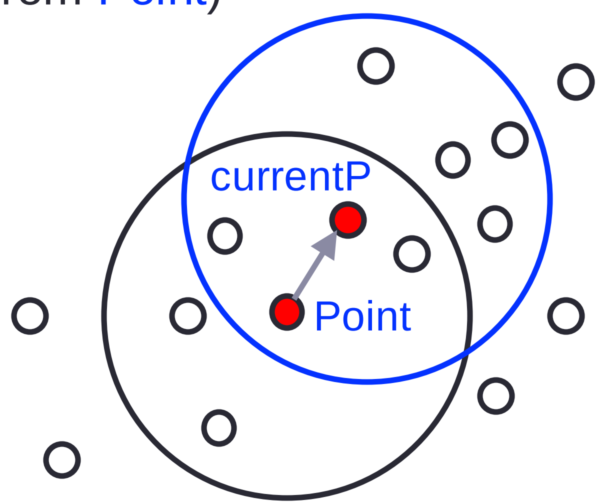

result = SetOfPoints.regionQuery()

result contains all the points in the Eps-neighborhood of currentP

we are scanning the second order Eps-neighborhood of Point

if result contains more than MinPts → continue, this set contains points that are all density reachable from currentP (and, in turn, from Point)



DBSCAN: ExpandCluster

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              IN {UNCLASSIFIED, NOISE} THEN
            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```

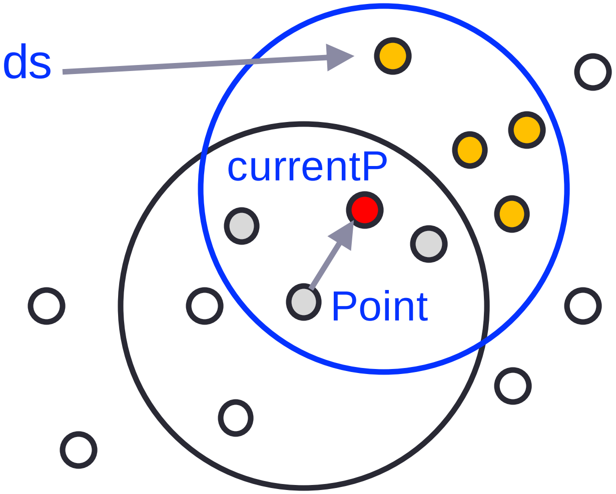
FOR each point in set result

If UNCLASSIFIED
→ add to set seeds

If UNCLASSIFIED or NOISE
→ change cluster ID with current ClId

NOTE: if the point is marked as NOISE we do not re-add it to seeds, as it was already processed, we only change its cluster ID

added to seeds



DBSCAN: ExpandCluster

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               MinPts) : Boolean;
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          resultP := result.get(i);
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            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```

NOTE: adding points to the seeds set reiterates the search by reaching all the points that are density connected through a path → assigning them the same cluster ID of the starting Point

DBSCAN: ExpandCluster

```
ExpandCluster(SetOfPoints, Point, ClId, Eps,
               MinPts) : Boolean;
  seeds:=SetOfPoints.regionQuery(Point,Eps);
  IF seeds.size<MinPts THEN // no core point
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      IF result.size >= MinPts THEN
        FOR i FROM 1 TO result.size DO
          resultP := result.get(i);
          IF resultP.ClId
              IN {UNCLASSIFIED, NOISE} THEN
            IF resultP.ClId = UNCLASSIFIED THEN
              seeds.append(resultP);
            END IF;
            SetOfPoints.changeClId(resultP,ClId);
          END IF; // UNCLASSIFIED or NOISE
        END FOR;
      END IF; // result.size >= MinPts
      seeds.delete(currentP);
    END WHILE; // seeds <> Empty
    RETURN True;
  END IF
END; // ExpandCluster
```
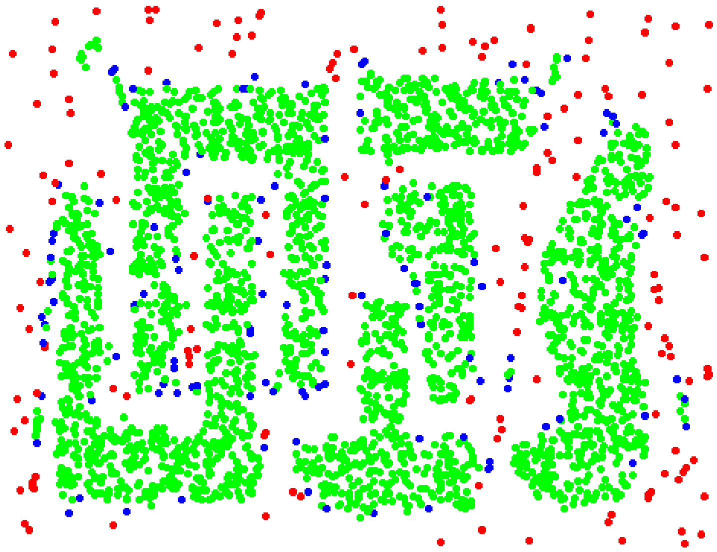

- delete currentP from seeds
- move to next point in seeds
- repeat until seeds is empty

2D example

original points

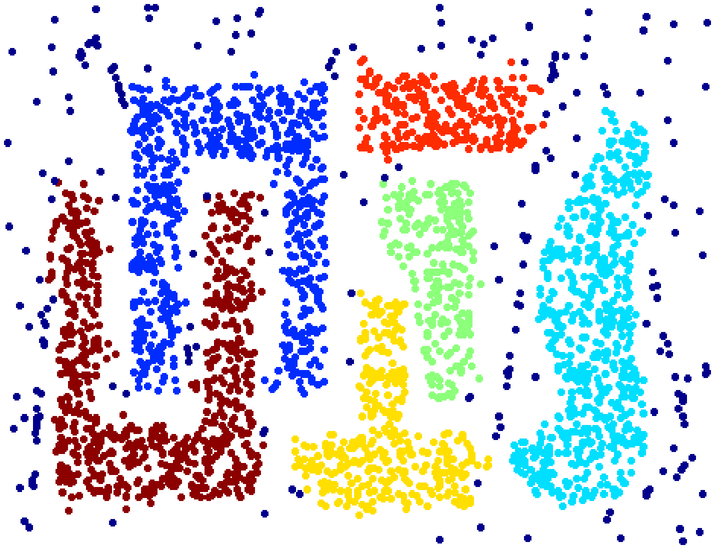


DBSCAN: **core points**, border & noise

Eps=10, MinPts=4

2D clustering result

original points



DBSCAN: clusters

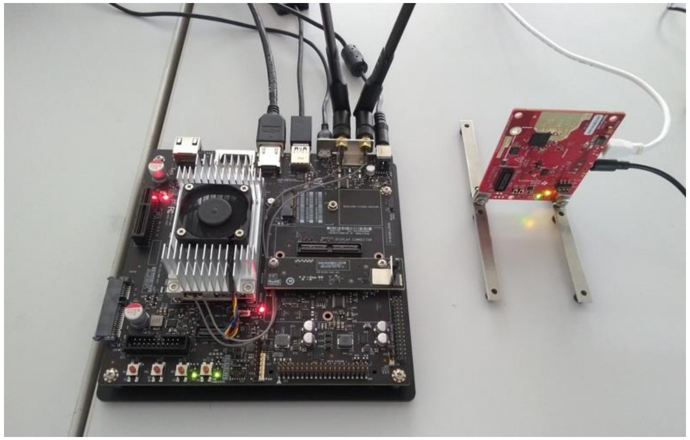
- DBSCAN works well
  - Resistant to noise
  - Handles clusters of different shape and size

DBSCAN complexity

- n: number of points to be clustered
- Time complexity: $O(n^2)$ – for each point it has to be determined if it is a core point. It can be reduced to $O(n*\log(n))$ in low dimensional spaces by using efficient data structures
- Space complexity: $O(n)$

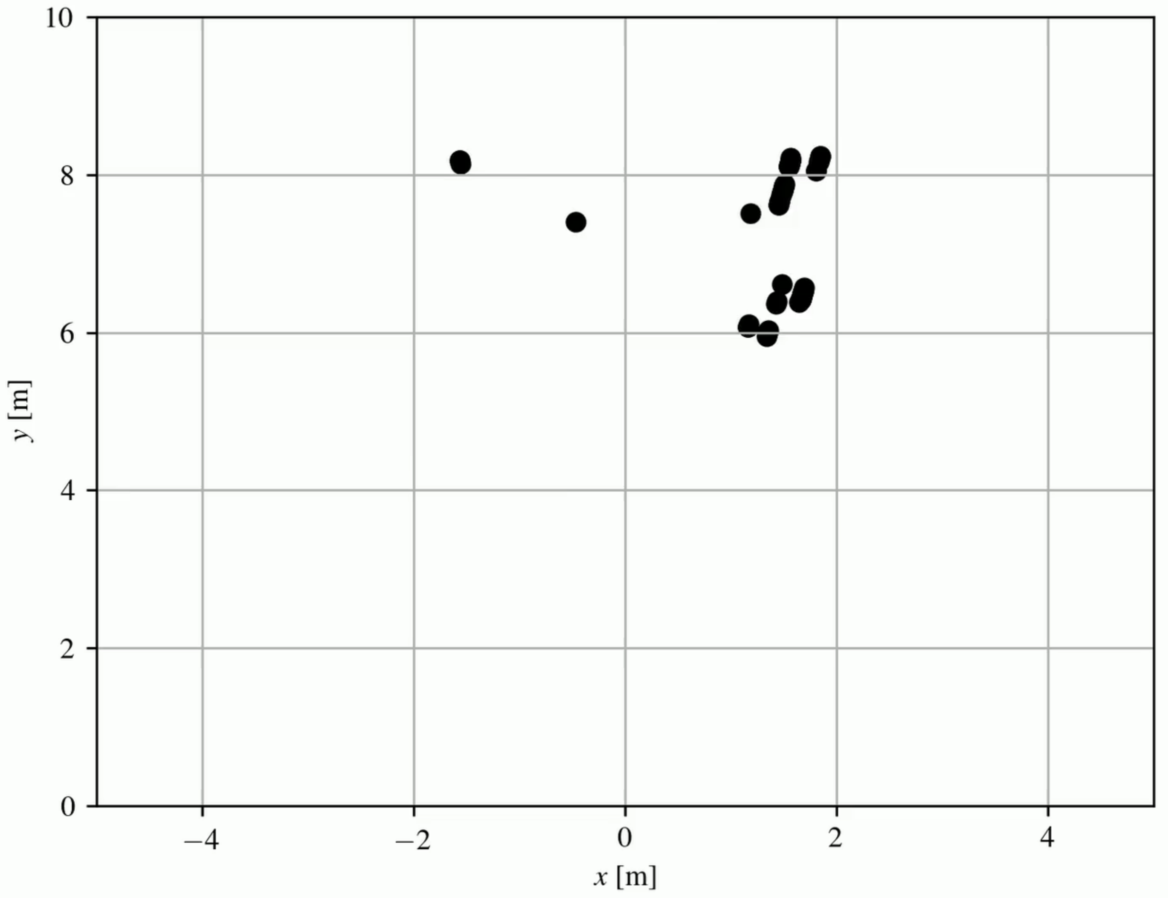
Practical example: mm-wave sensing

- IWR1843 single-chip 76-GHz to 81-GHz industrial radar
  - FMCW radar, 76 to 81 GHz (4GHz bandwidth)
  - Evaluation board from Texas Instruments
  - Cortex R4F micro-controller for object tracking
  - Antennas: 3(TX), 4(RX)

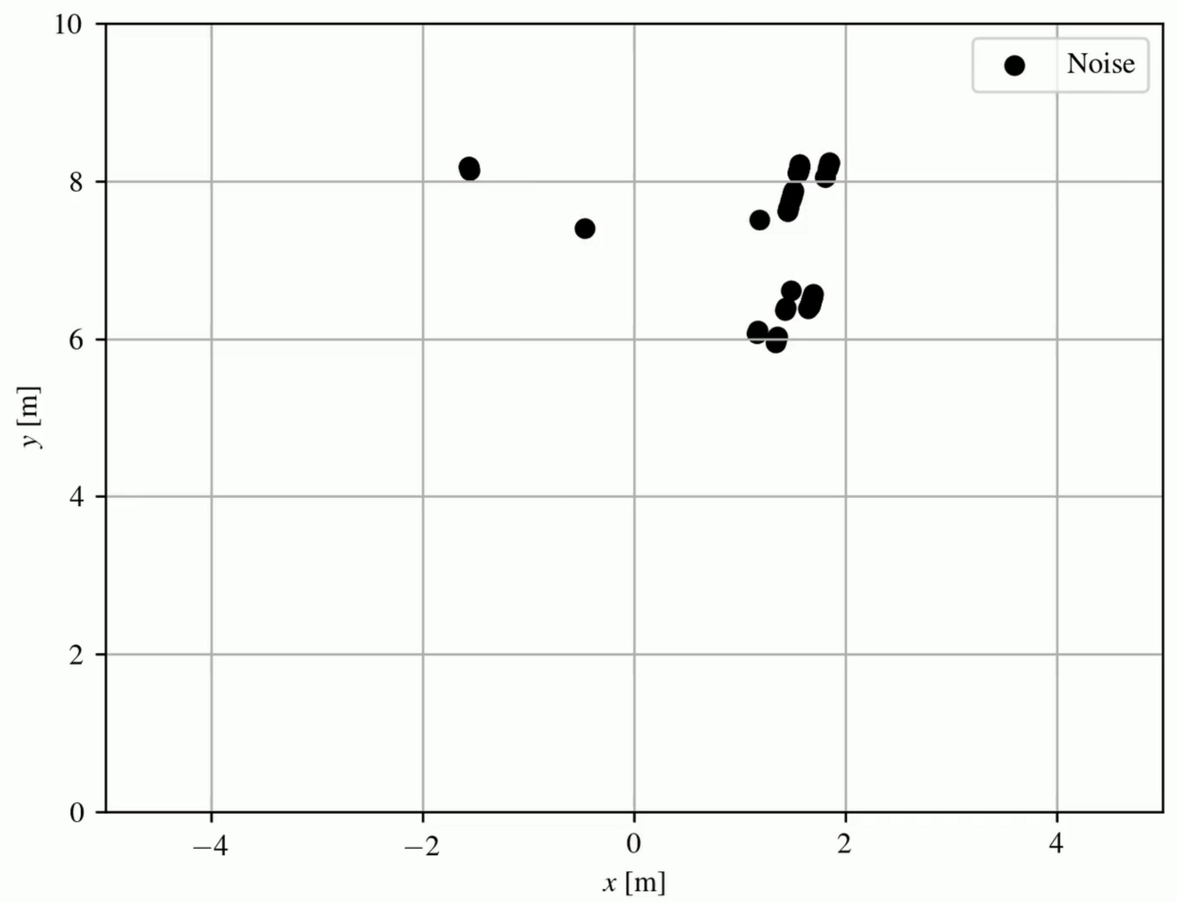


NVIDA Edge Computer (Jetson TX2)

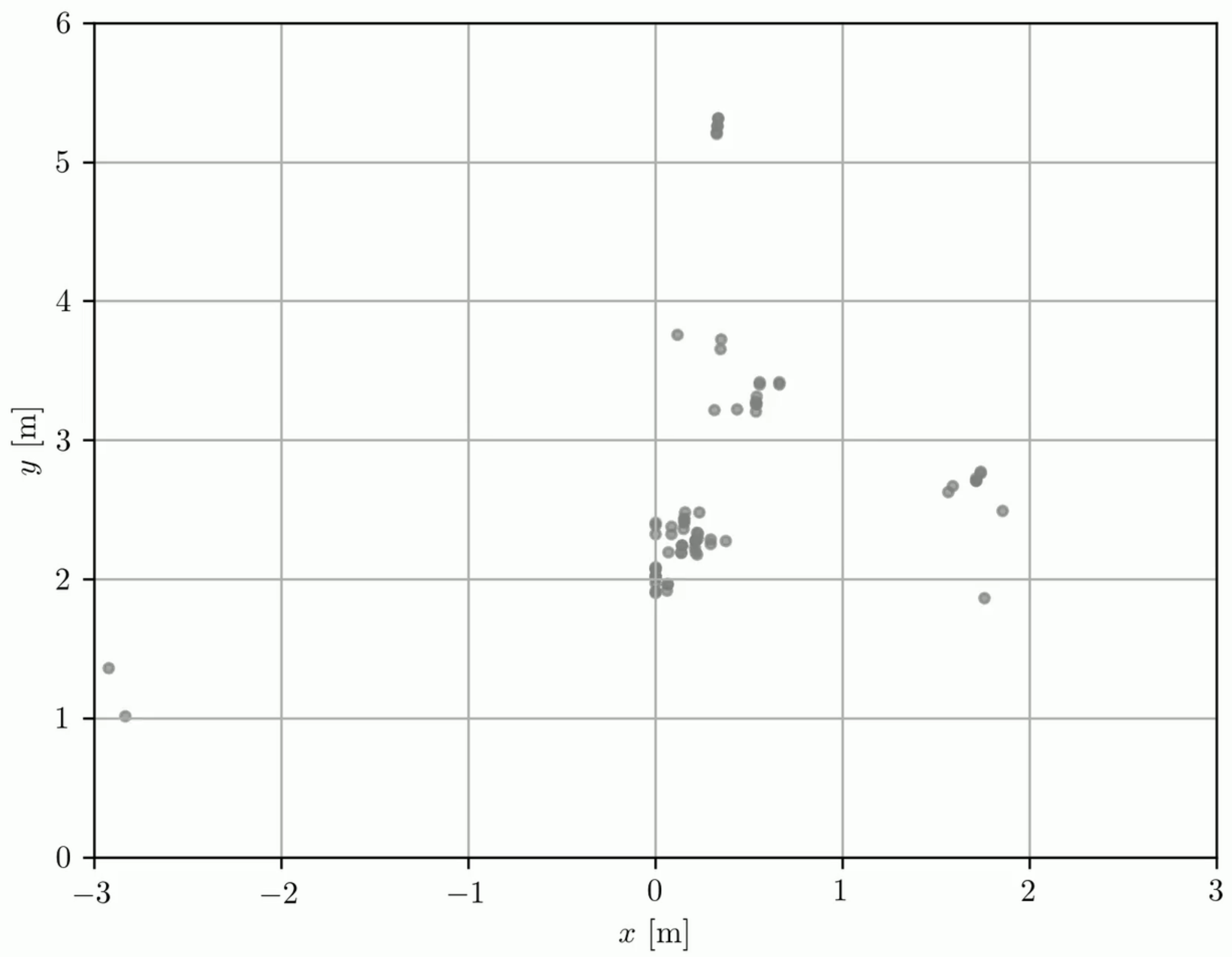
Raw data: mm-wave point cloud



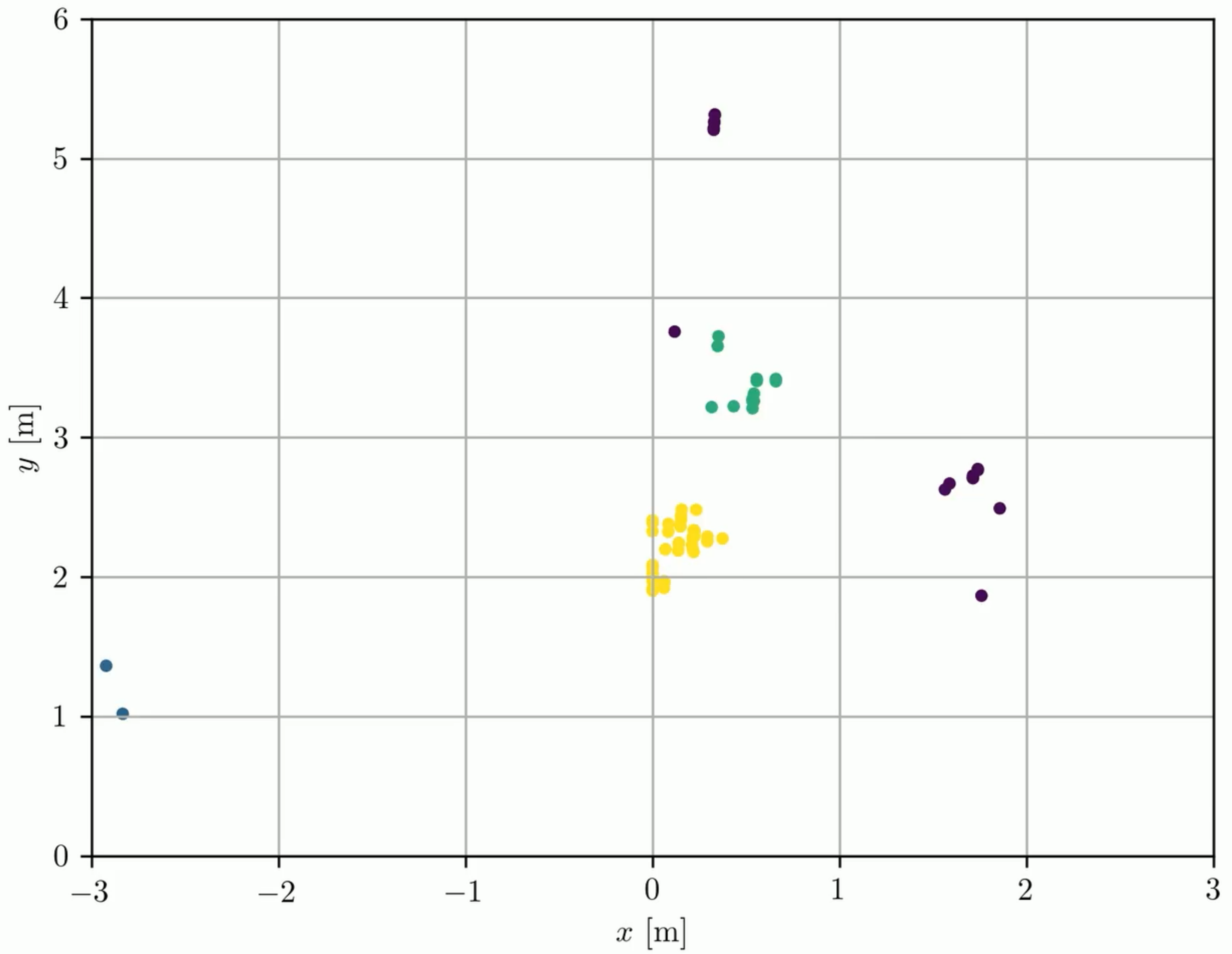
DBSCAN applied to point clouds



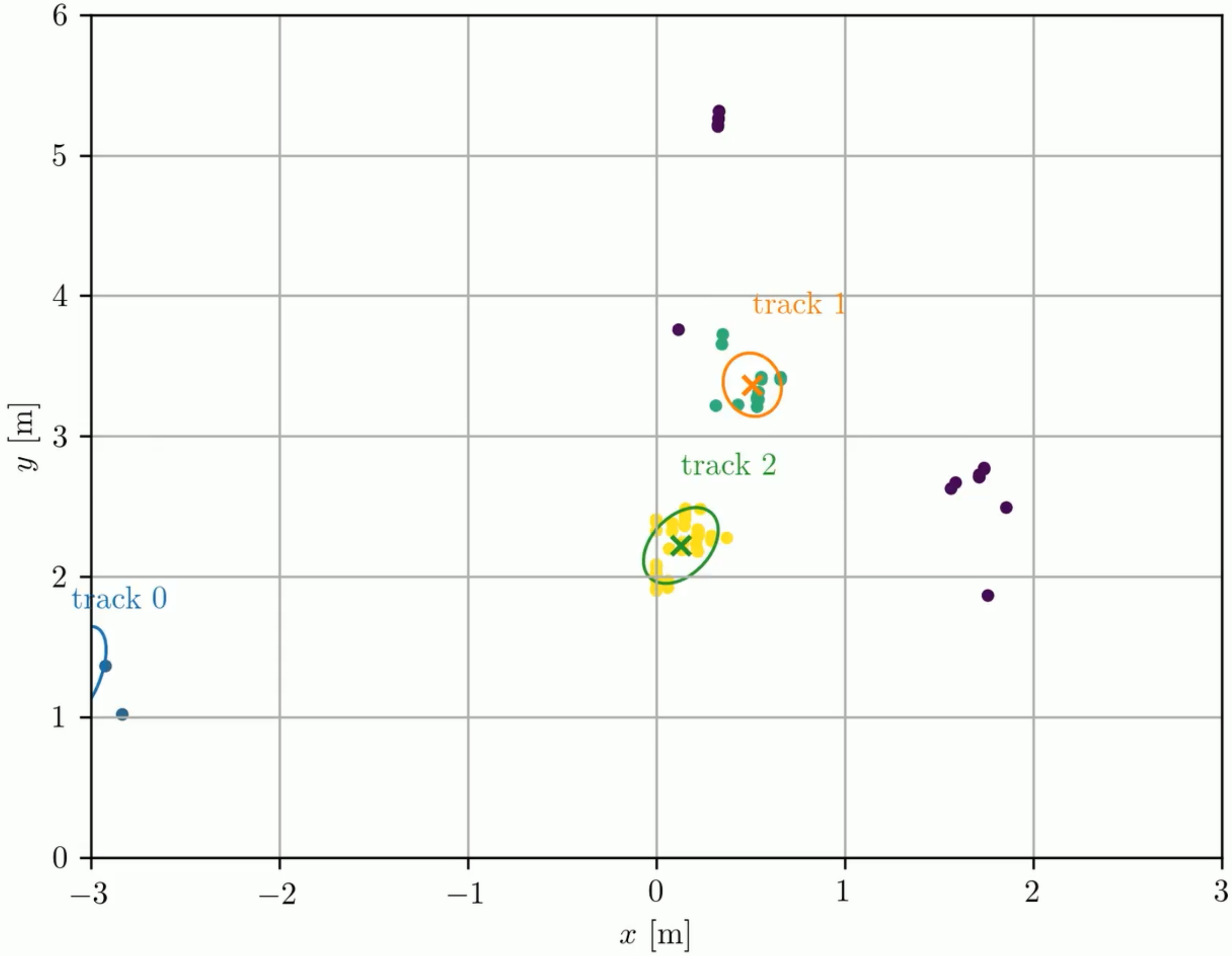
Raw point clouds from the radar



DBSCAN clusters



After some more magic…



Setting MinPts

- Is there an exact method? No, it is heuristic, and emprirical…

- The larger the data set, the larger the MinPts variable should be
- If the data set is noisier, choose a larger value of MinPts
- Guidelines from experiments
  - Generally, MinPts should be greater than or equal to the dimensionality of the data set
  - For 2-dimensional data, default value of MinPts = 4 [Ester1996]
  - If your data has more than 2 dimensions, choose MinPts = 2*dim, where dim= the dimensions of your data [Sander1998]

[Sander1998] X. Xu, M. Ester; H.-P. Kriegel, J. Sander, A distribution-based clustering algorithm for mining in large spatial databases, Int. Conference on Data Engineering, February 1998.

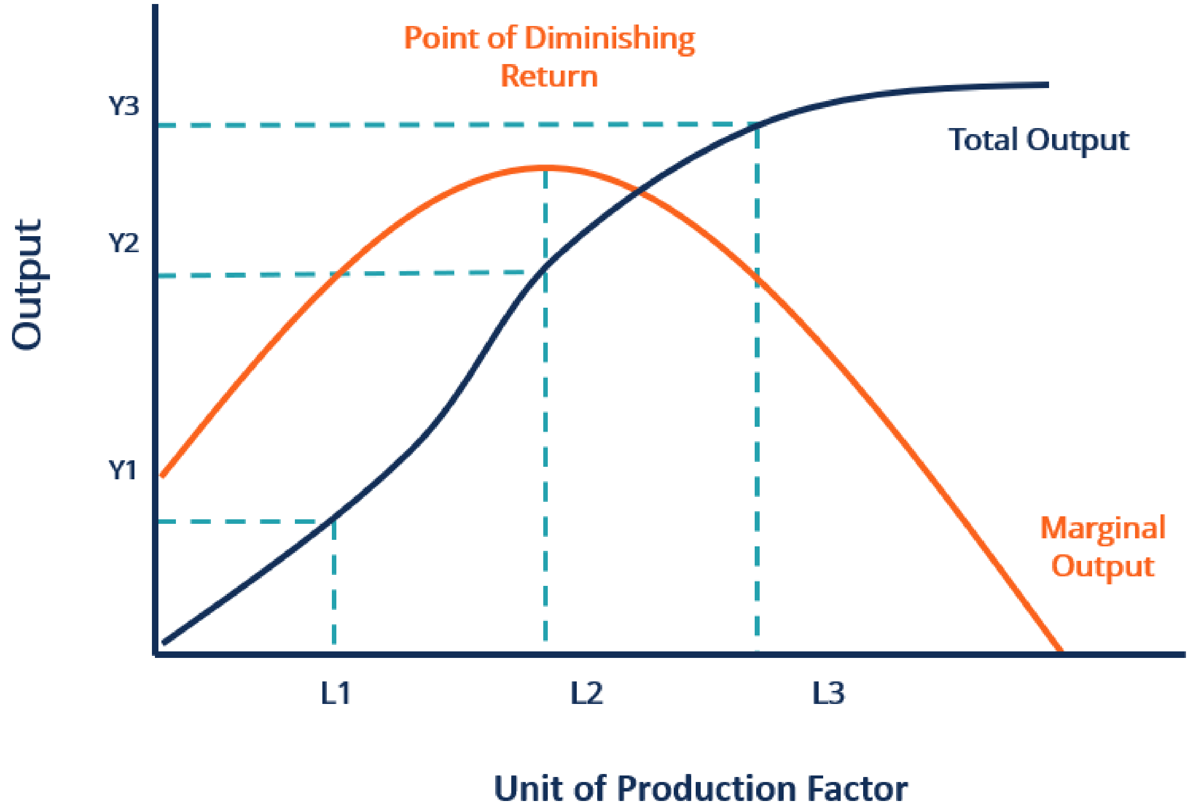
Dimishing returns (microeconomics)

Production process

- As production factor increases (e.g., workforce), the total output also increases
- At some point, however, it will reach an optimal output level, after which the output flattens or decrease
- Production factors = labor, machine hours, raw material

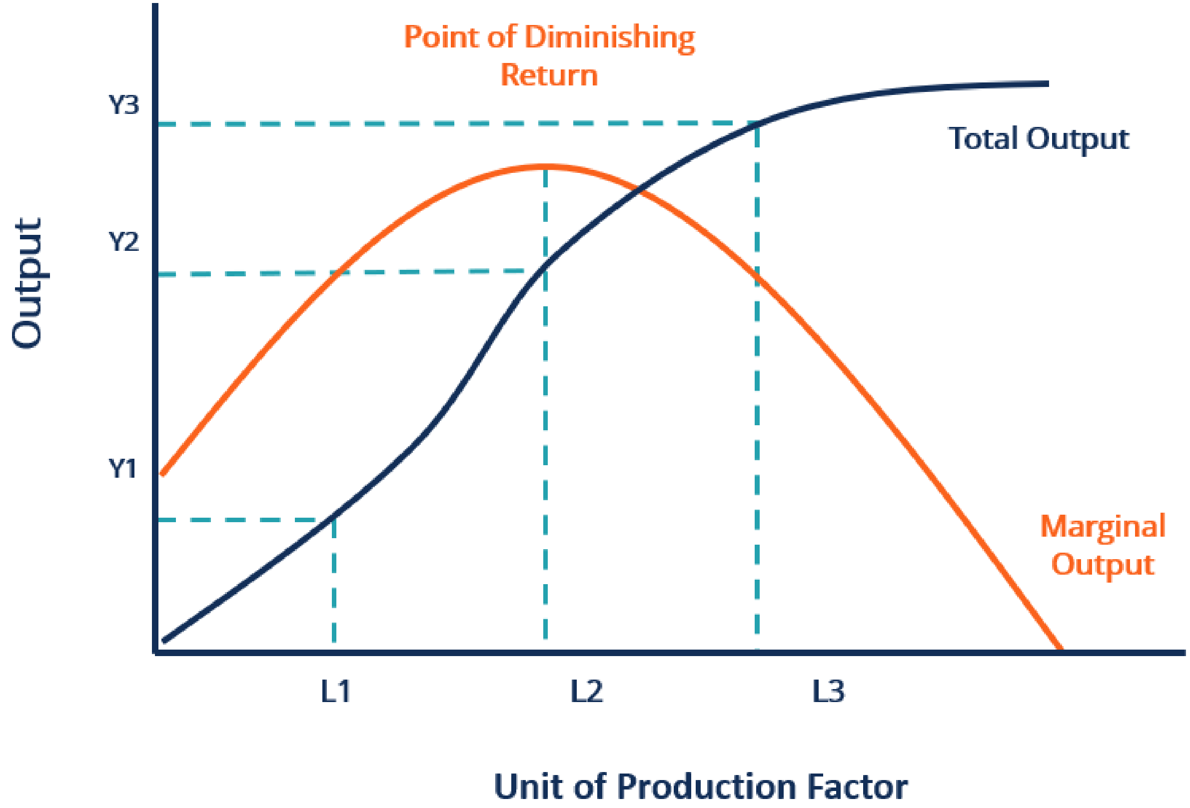
"Assuming a constant level of other production factors, every additional unit of a production factor leads to a greater increase in total output (marginal output) initially. After reaching a certain optimal production level, every additional unit of the production factor will result in a smaller increase in total output with a diminishing marginal output, as the efficiency is limited by the other production factors…"

Dimishing returns



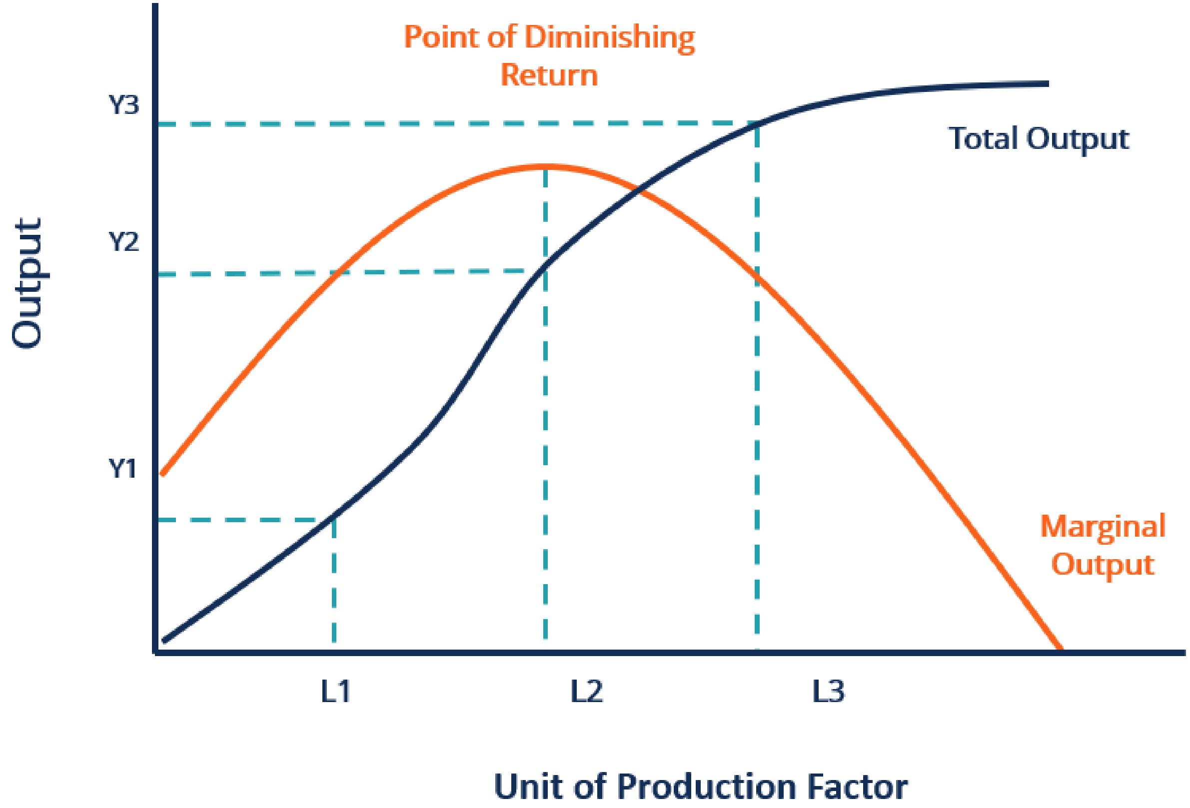
If production factor increases from L1 → L2, the increase in the output is Y2-Y1, this is called marginal return

Dimishing returns



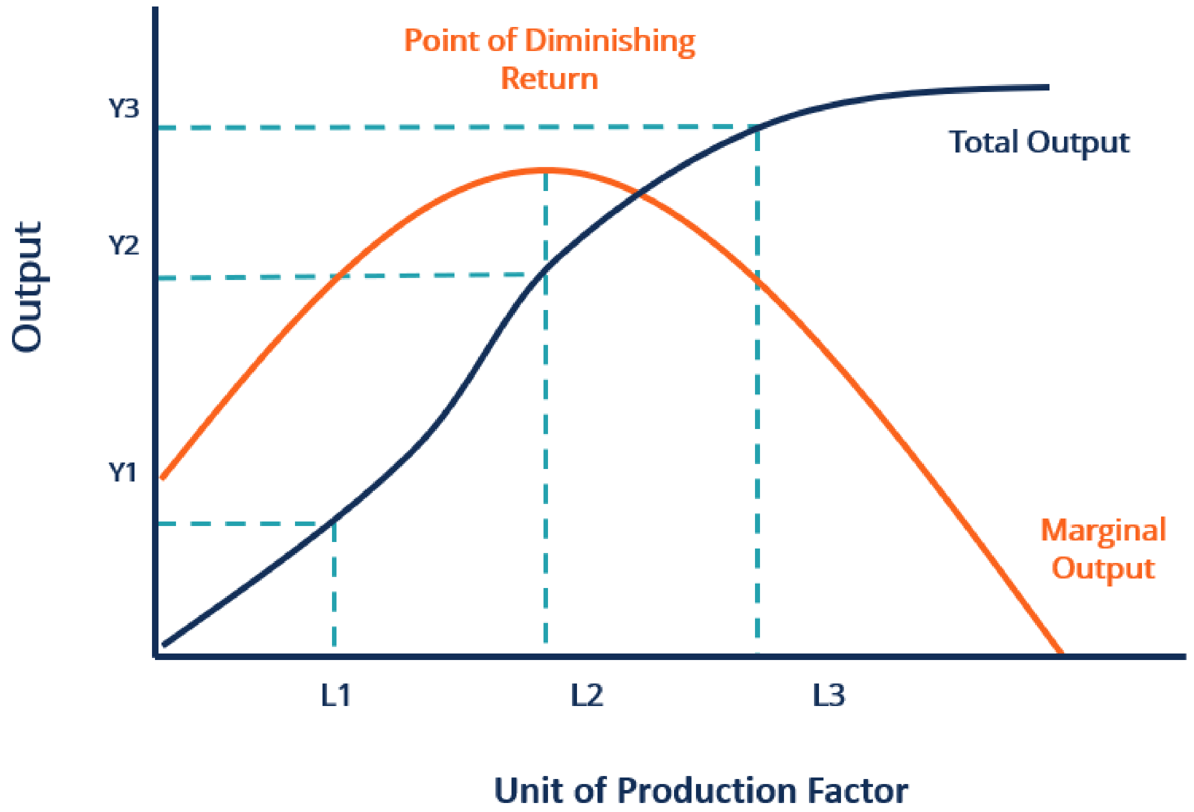
If production factor increases from L2 → L3, the marginal return is Y3-Y2, which is smaller than Y2-Y1

Dimishing returns



If production factor keeps increasing the marginal return eventually goes to zero

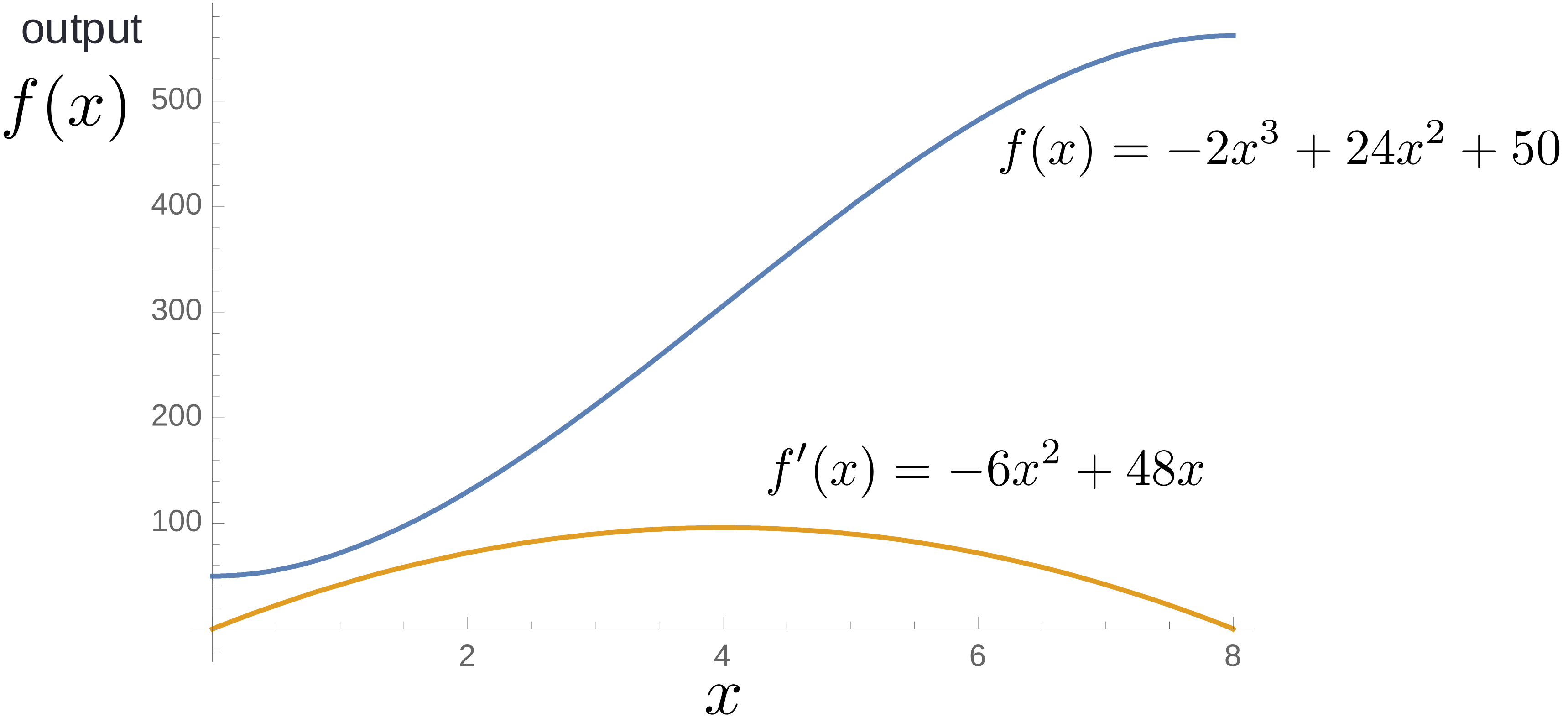
Dimishing returns



The point where the marginal return is maximum is L2

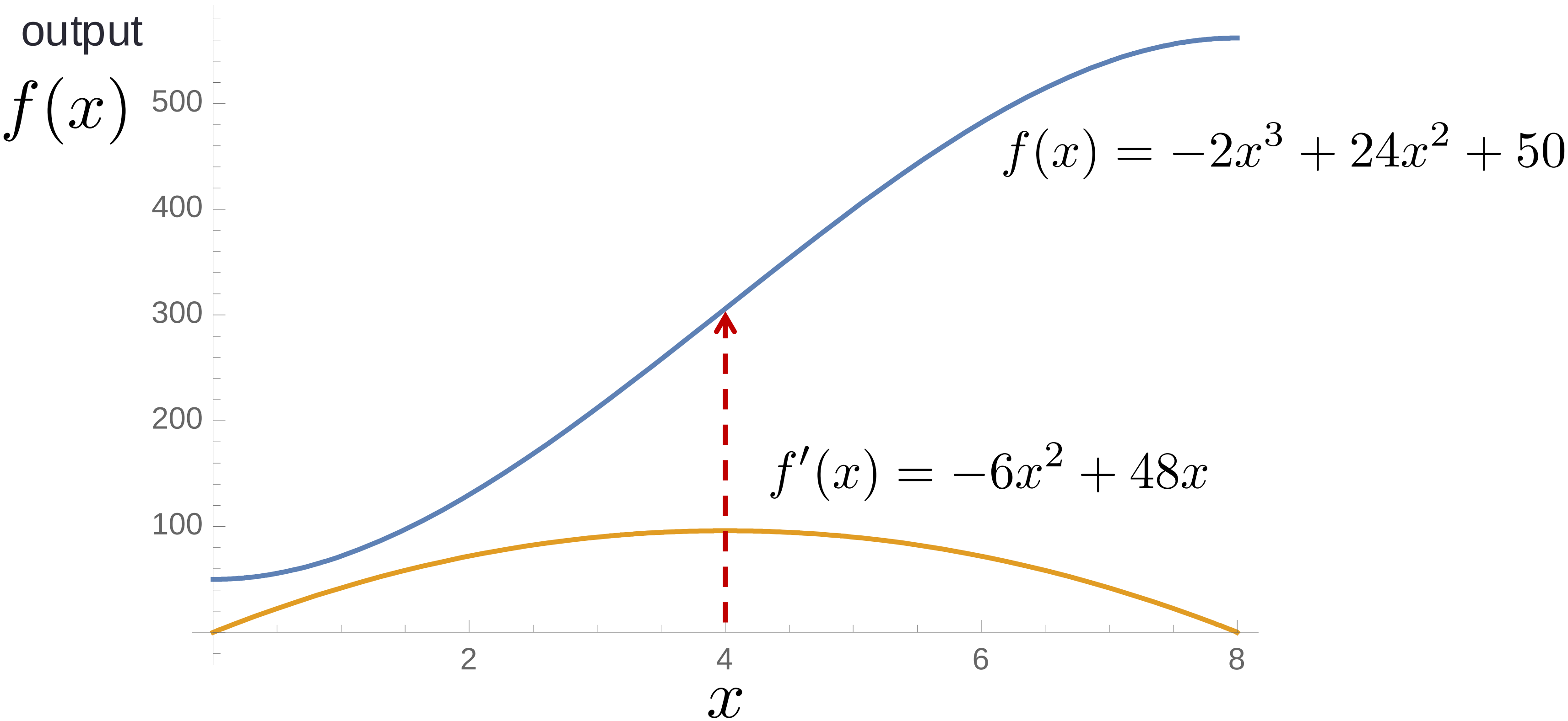
How do we find it?

Marginal returns example



We look at the first order derivative of the output as a function of the production factor

Marginal returns example

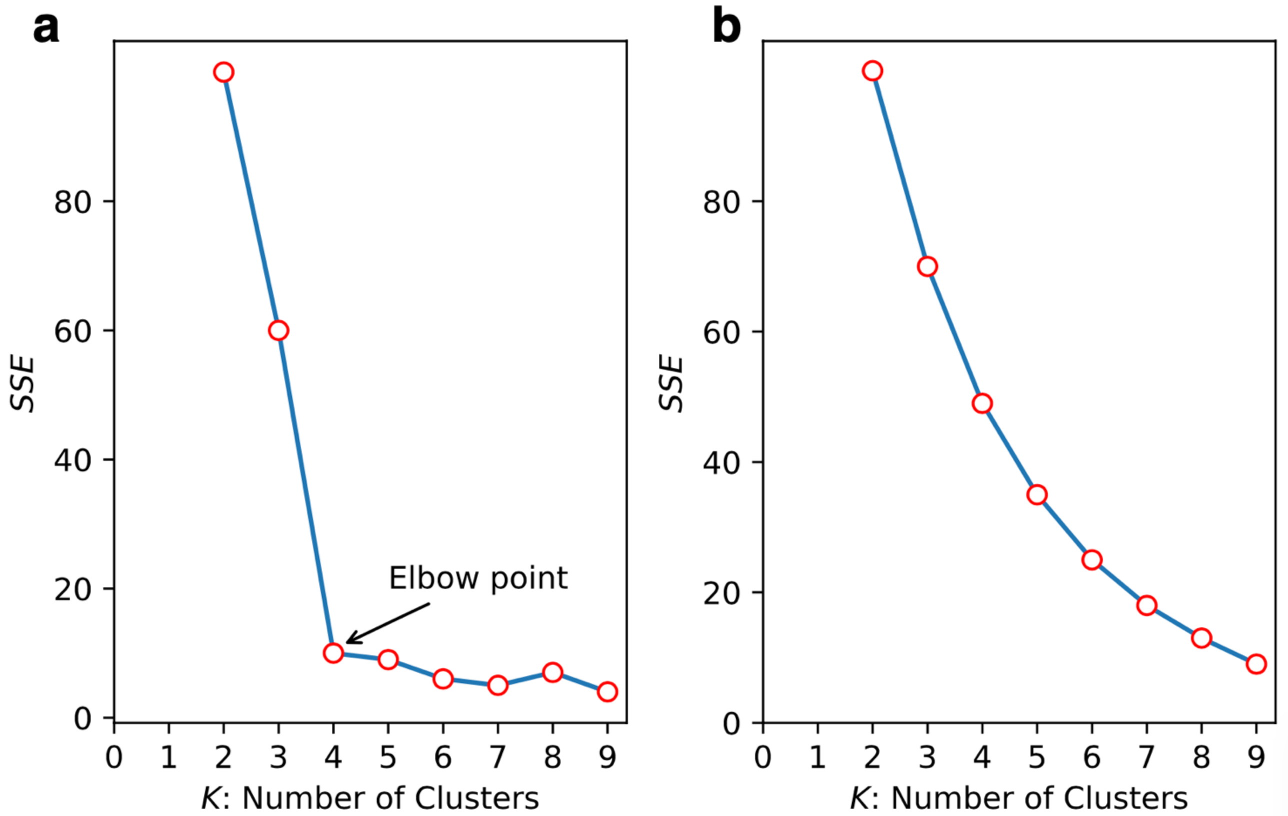


The maximum marginal return is achieved when the first order derivative is maximum, or when the second order derivative is zero (inflection point of f(x))

Clustering – choice of K? (e.g.. K-means)

SSE = Sum of Squared Distances $SSE = \sum_{k=1}^{K} \sum_{\boldsymbol{x}_i \in \mathcal{C}_k} \|\boldsymbol{x}_i - \boldsymbol{\mu}_i\|^2$

SSE for two datasets **a** & **b**



Knee detection

- Problem: *“finding the inflection point can be done analytically for continuous analytical functions, for which the first (and second) order derivatives can be analytically computed. It is much harder to compute it for empirical curves obtained from discrete data points (domain of x is discrete and points are not equally spaced) – this is often the case in practice”*
- Possible solution: “Kneedle” [Satopää2011], a heuristic algorithm that robustly works with experimental datasets

[Satopaa2011] V. Satopää, J. Albrecht, D. Irwin, B. Raghavan, A "Kneedle" in a Haystack: Detecting Knee Points in System Behavior, Int. Conference on Distributed Computing Systems, 2011. [1251 citations. October 2024]

A simple but effective algorithm

- In [Satopaa2011], the “elbow” points are detected as apoint of maximum curvature of f(x)
- Curvature of f(x), continuos with 1st & 2nd order derivatives

$$K(x) = \frac{|f''(x)|}{[1 + f'(x)^2]^{3/2}}$$

- The point of max curvature is

$$x^\star = \operatorname*{argmax}_x K(x)$$

[Satopaa2011] V. Satopää, J. Albrecht, D. Irwin, B. Raghavan, A "Kneedle" in a Haystack: Detecting Knee Points in System Behavior, Int. Conference on Distributed Computing Systems, 2011.

A simple but effective algorithm

- Problem
  - Curvature is not well-defined for discrete (and noisy) functions
  - And it is difficult to approximate considering the analytical equation

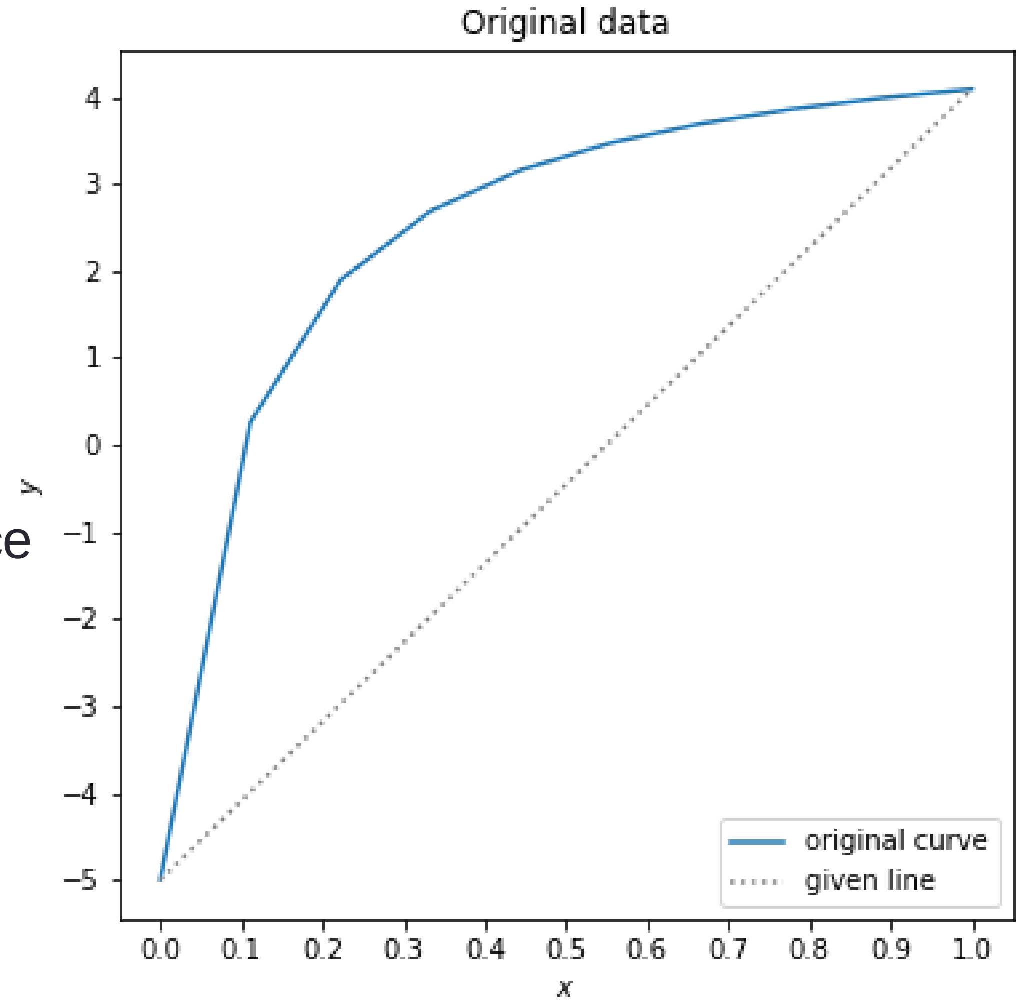
[Satopaa2011] V. Satopää, J. Albrecht, D. Irwin, B. Raghavan, A "Kneedle" in a Haystack: Detecting Knee Points in System Behavior, Int. Conference on Distributed Computing Systems, 2011.

1. Original data

Kneedle by example

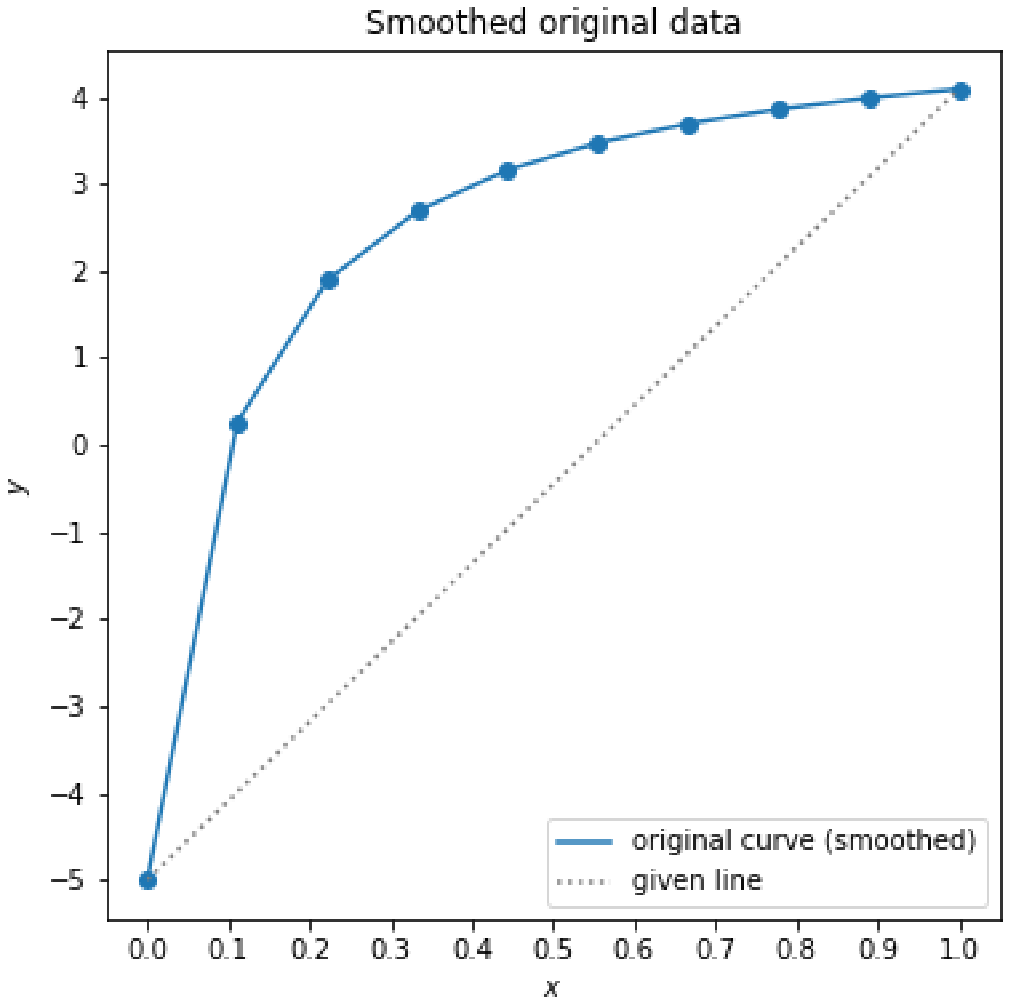
- Pragmatic approach
- Plot quality measure
  - Possibly rotated
- Can be
  - K-means: distortion J *vs* K
  - DBSCAN: average distance in neighborhood *vs* points

  …



2. Smooth data

- Smooth data
  - e.g. using splines (among many options)



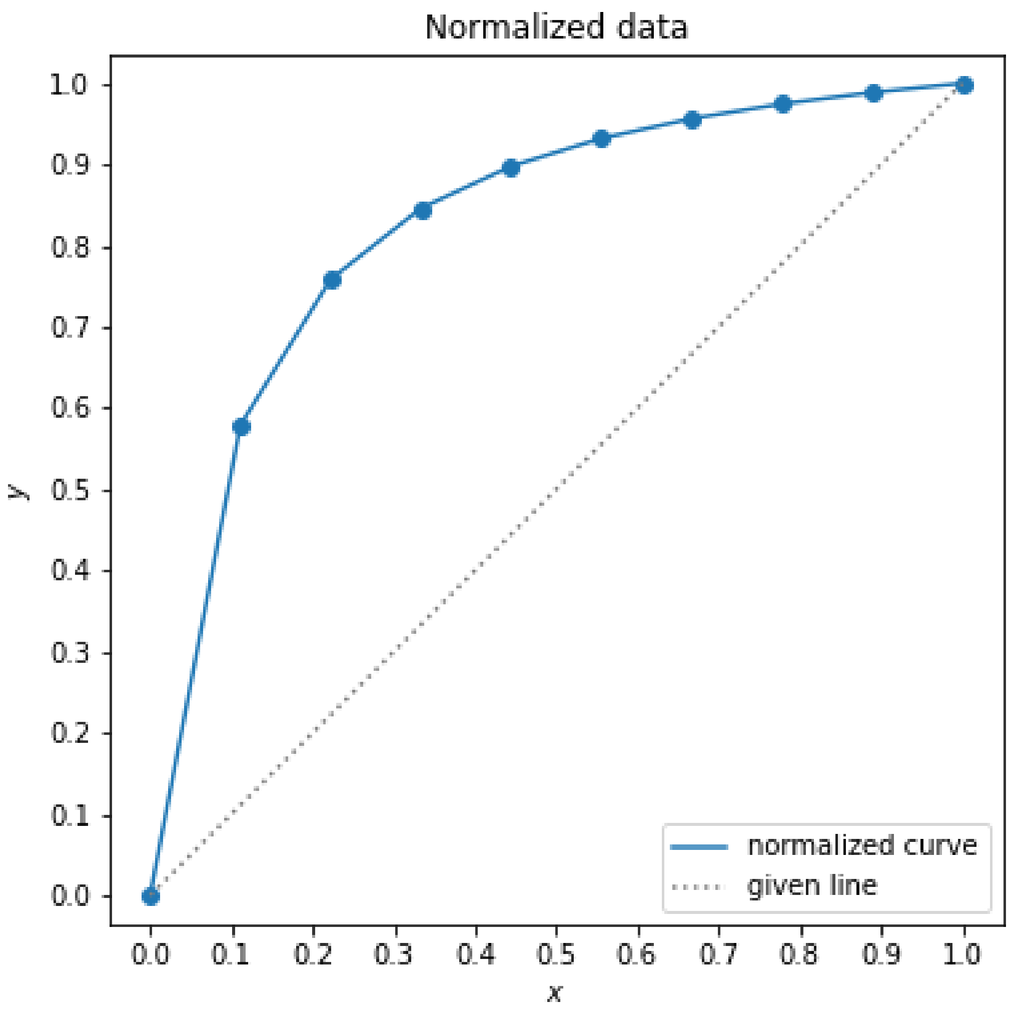
3. Normalize data

- Both axes in [0,1]

Transformation

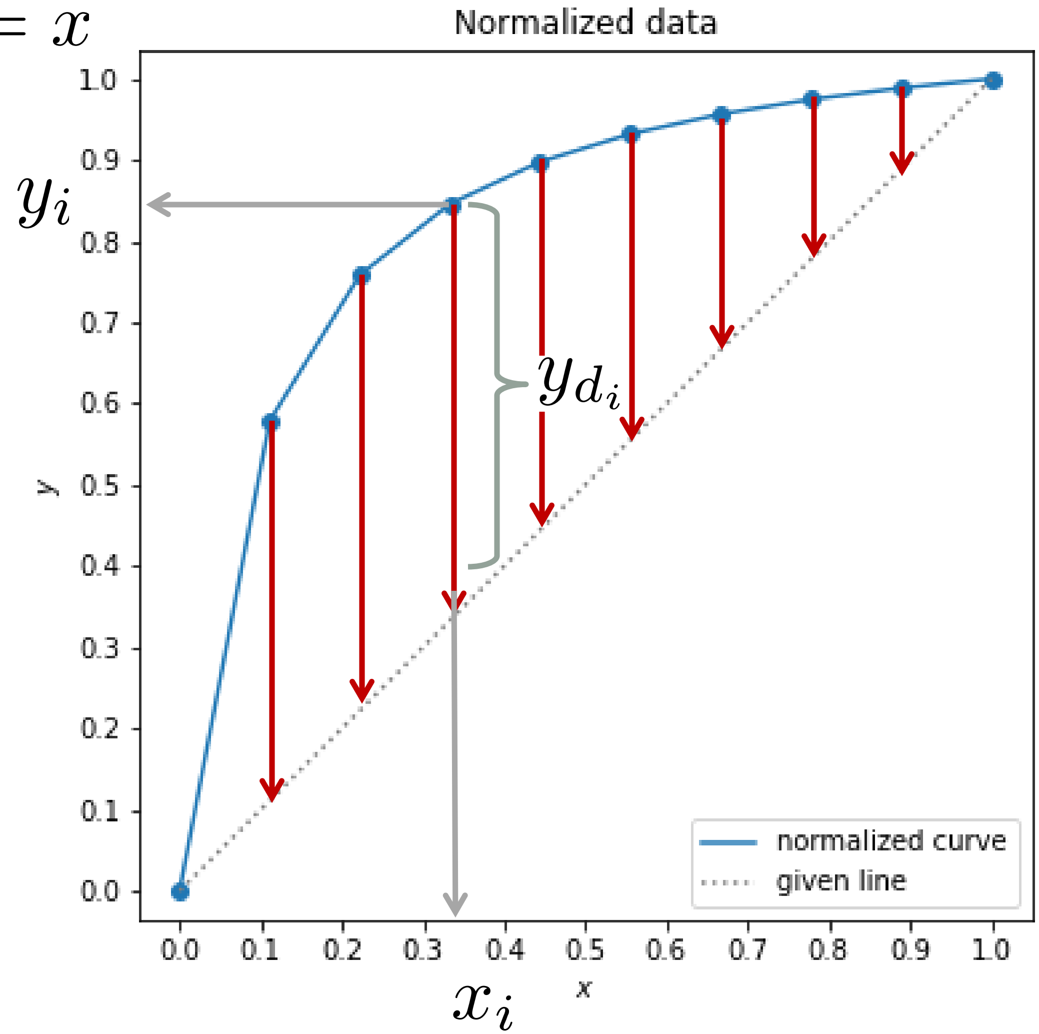
$$x_i \leftarrow \frac{x_i - x_{\min}}{x_{\max} - x_{\min}}$$

$$y_i \leftarrow \frac{y_i - y_{\min}}{y_{\max} - y_{\min}}$$



4. Calculate distances from y=x line

- With respect to line $y = x$ such distances are related to the local value of the curvature of f(x)



Note:

- the curvature measures how much a curve deviates from a straight line
- hence, y_{d_i} is a good proxy to the curvature metric

5. Plotting such distances

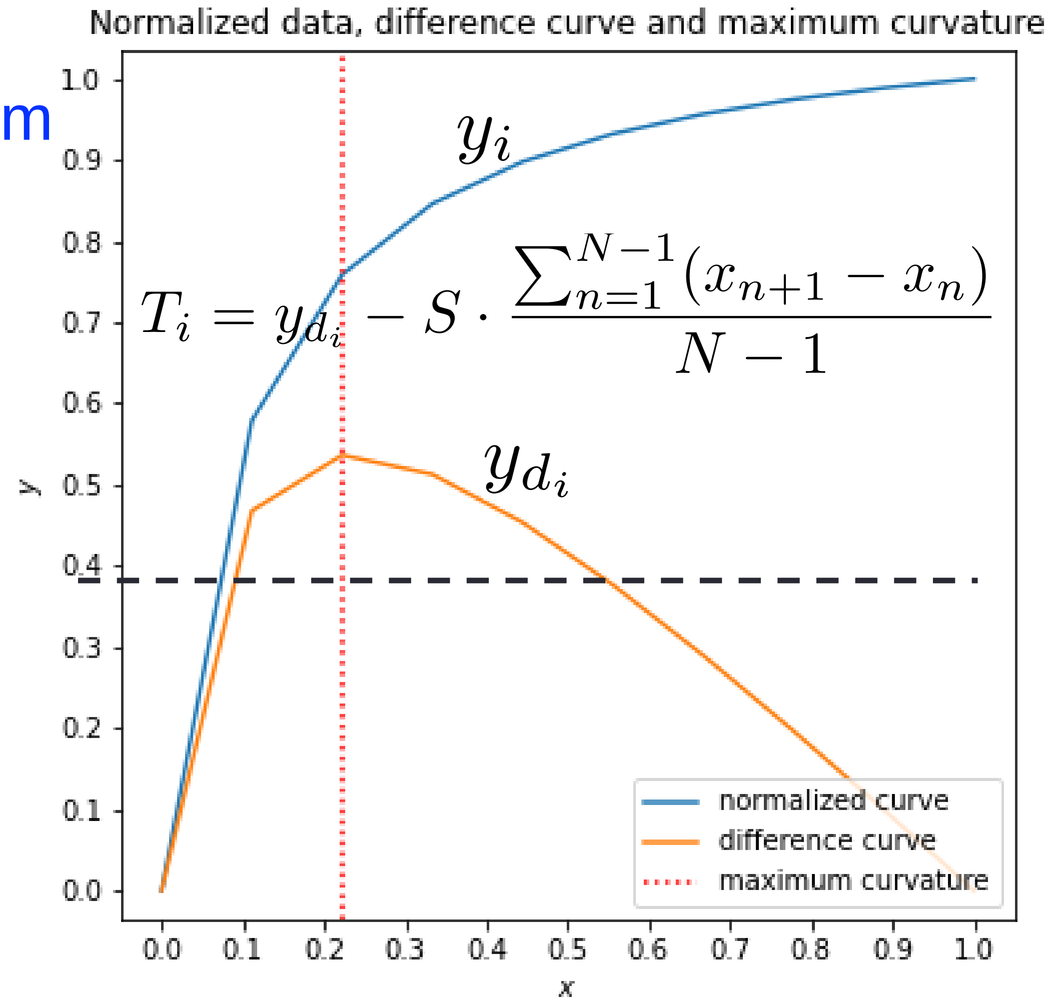
Assume:

(x_i, y_{d_i}) is a local maximum

y_{d_i} difference value for x_i

A threshold T_i is defined for each local maximum candidate

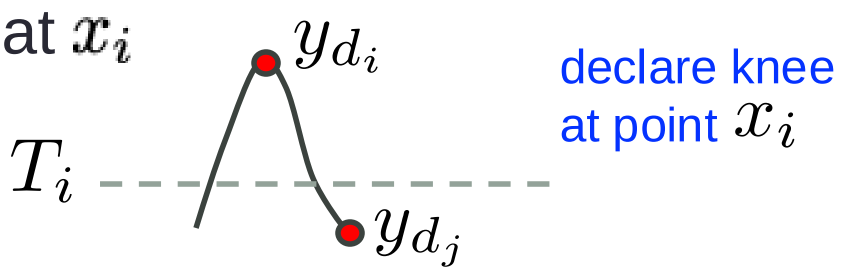
S is a *sensitivity* par (e.g., S=1) – to declare the maximum (tunable)



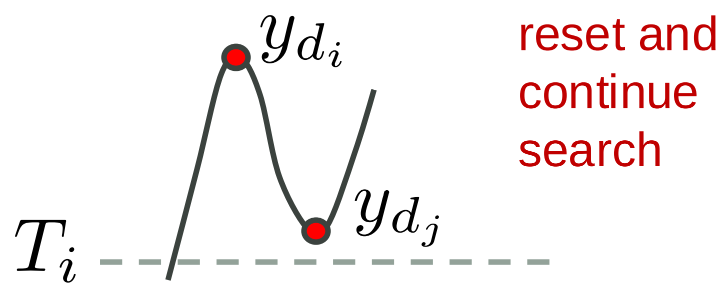
Locating maxima

If (x_i, y_{d_i}) is a local maximum

- If any subsequent value (x_j, y_{d_j}) with $j > i$ drops below T_i before the next local maximum in the difference curve is reached, a Knee is declared at x_i



- If (x_j, y_{d_j}) reach a local minimum and start to increase before reaching T_i we reset the threshold to 0 and wait for another local maximum to be reached



Threshold meaning

$$T_i = y_{d_i} - S \cdot \boxed{\frac{\sum_{n=1}^{N-1}(x_{n+1} - x_n)}{N-1}}$$

average distance of two subsequent points

S: is a measure of how many (subsequent) flat points in the original curve we expect to see before declaring a knee

Note: is the original curve is flat as we move from $x_i \rightarrow x_{i+1}$ it holds

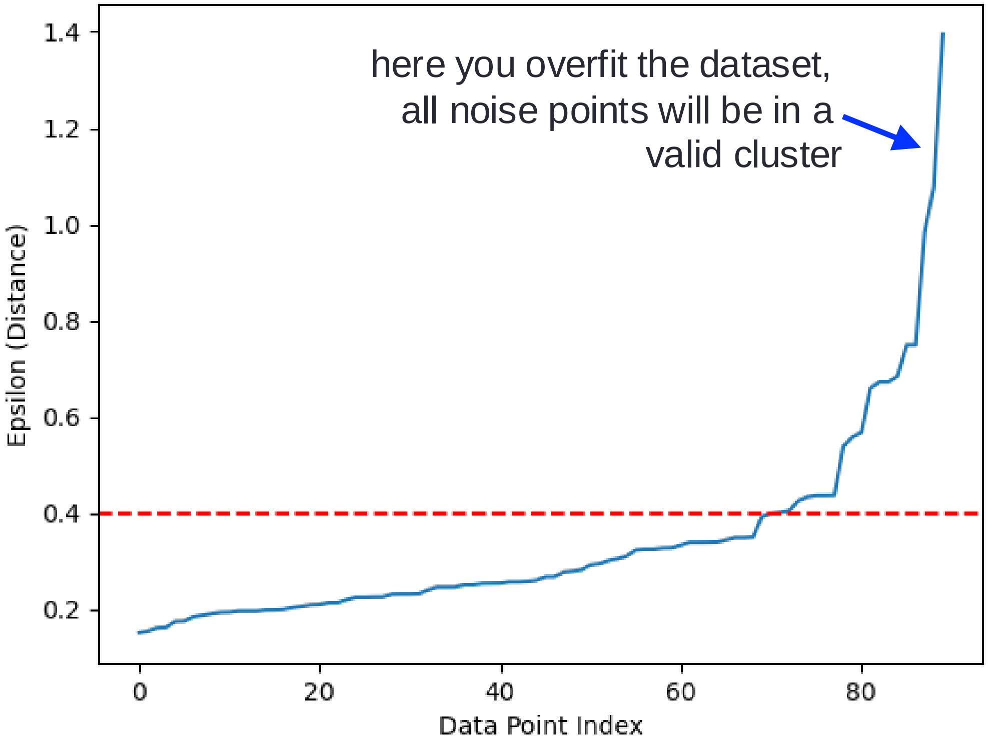
$$\Delta y_{d_i} = y_{d_{i+1}} - y_{d_i} = x_{i+1} - x_i$$

The threshold is

$$T_i = y_{di} - S \cdot \overline{(x_{n+1} - x_n)}$$

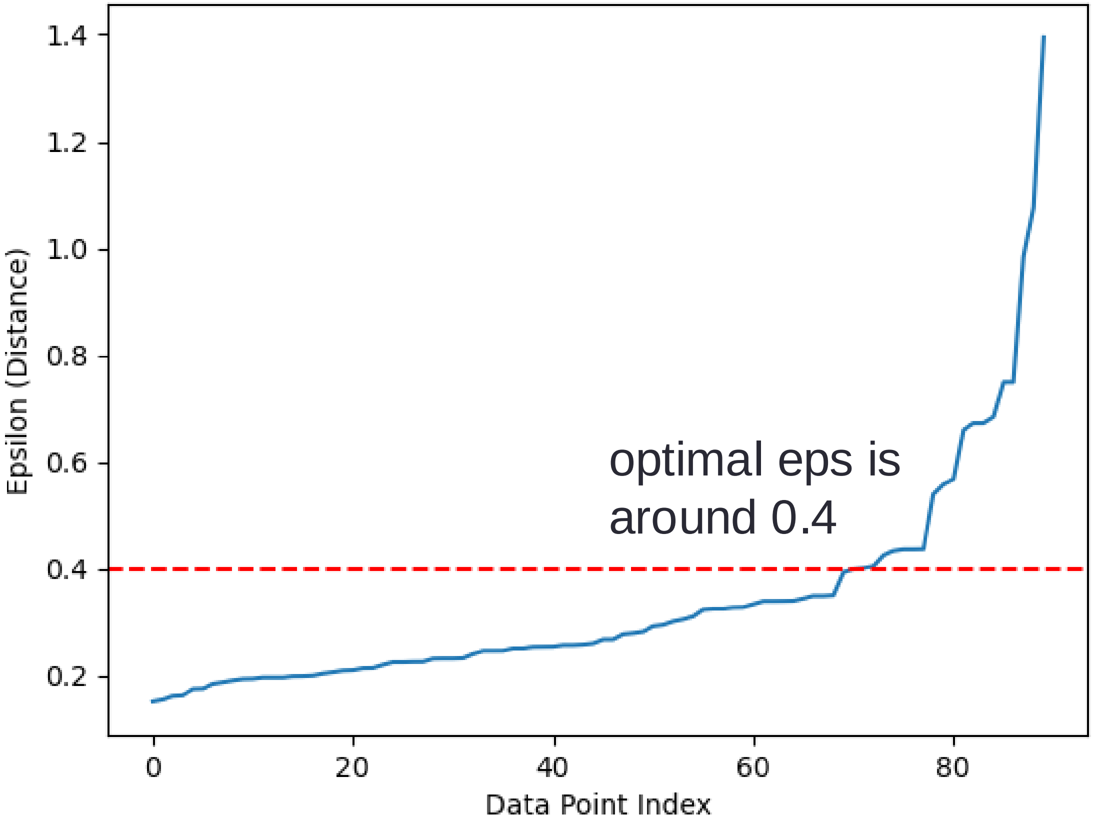
DBSCAN

- **For each point:** measure distance from its MinPts neighbors (all the points in the ε-neighborhood), compute & plot the average of it
- Order points based on such distance (ascending order)
- Plot distances for all points (ascending order)



DBSCAN

- Flip, smooth and normalize the curve
- Locate the optimal ε using Kneedle

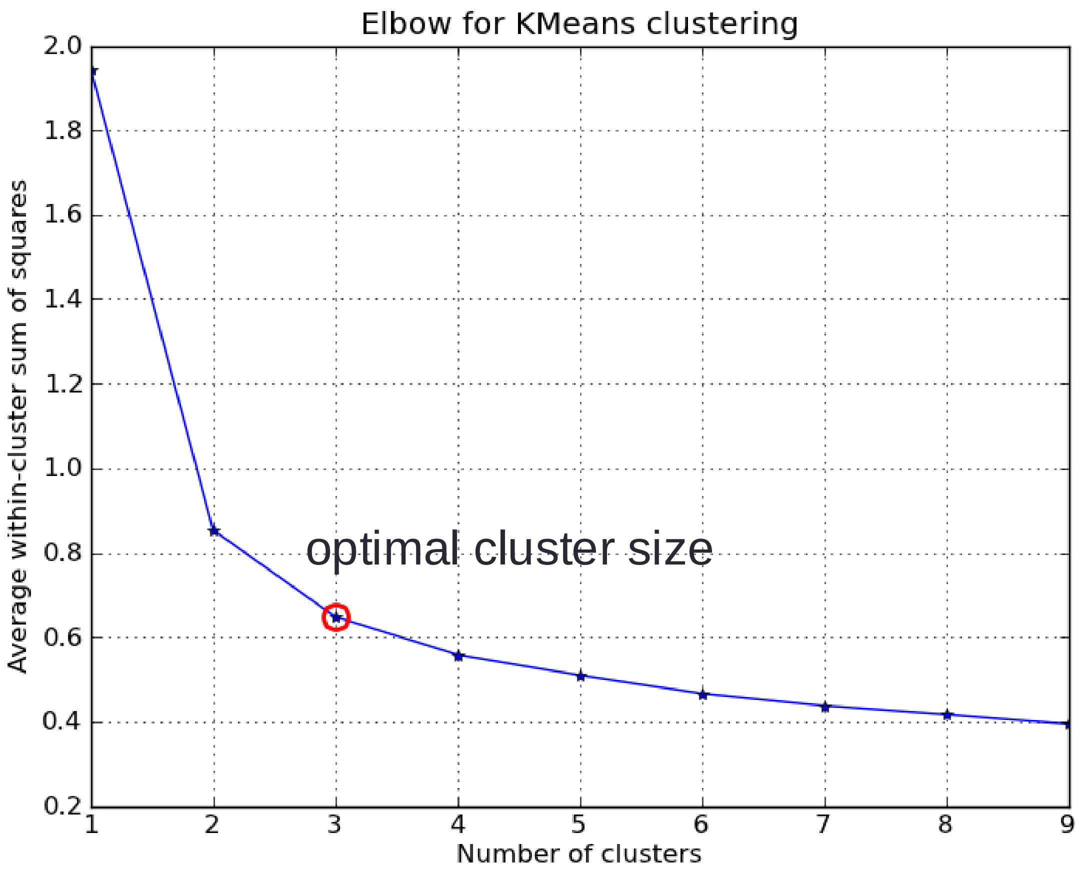


Clustering – selection of K

- Plot distortion measure (e.g., sum of distances from centroids)
- Look for inflection point
- Kneedle still applies
- Just replot using

$$y_i \leftarrow y_{\max} - y_i$$

- Smooth
- Normalize in [0,1]



Python libraries

- Kneed
  - https://github.com/arvkevi/ikneed
- Kneebow
  - https://pypi.org/project/kneebow/

Master's degree ICT Internet Multimedia Engineering

DENSITY BASED CLUSTERING: DBSCAN

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