k-Nearest Neighbors.
Local Learning.
Curse of Dimensionality.

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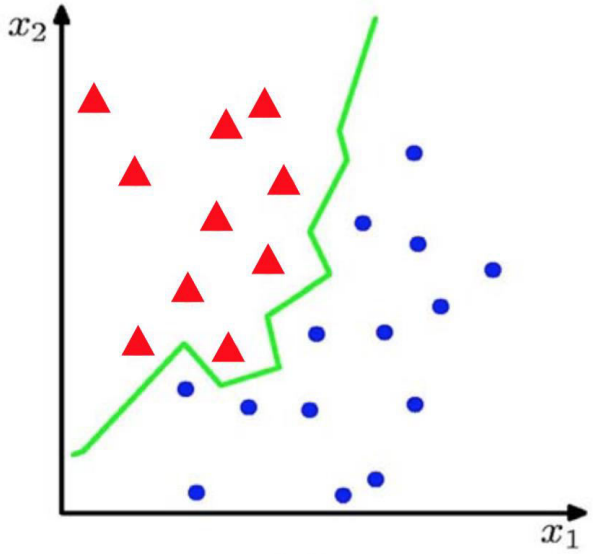
Classification from labeled samples



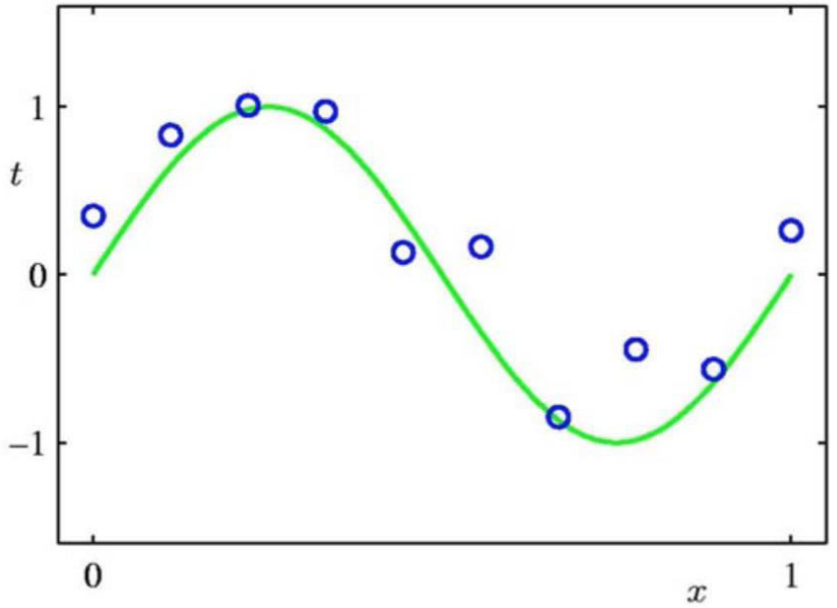
- Suppose we have a set of N training examples:

$$(x_1, \ldots, x_N) \text{ and } (y_1, \ldots, y_N), x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$$

- The classification problem consists of estimating the function g(x) such that:

$$g(x_i) = y_i$$

Regression from labeled samples



- Suppose we have a set of N training examples:

$(x_1, \ldots, x_N)$ and $(y_1, \ldots, y_N), x_i, y_i \in \mathbb{R}$

- The regression problem consists of estimating the function g(x) such that:

$$g(x_i) = y_i$$

Learning from labeled samples

- Suppose we have a set of N training examples:

$$(x_1, \ldots, x_N) \text{ and } (y_1, \ldots, y_N), x_i, y_i \in \mathbb{R}$$

- The learning problem consists of estimating g(x) such that:

$$g(x_i) = y_i$$

- The loss function (e.g. MSE):

$$\mathcal{L}(y, g(\mathbf{x}))$$

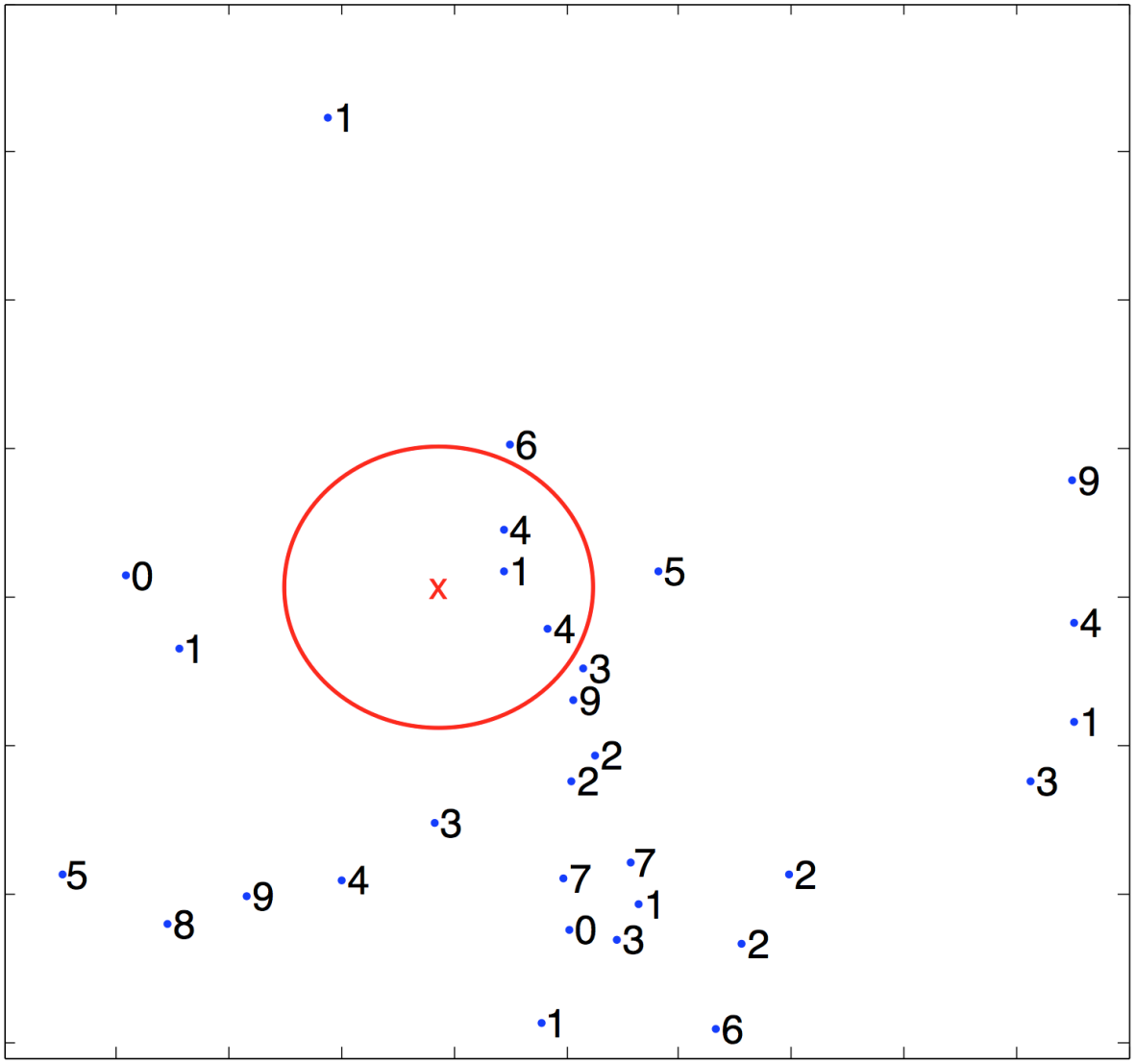
- Generalization error:

$$L(g) = E_P \mathcal{L}(y, g(\mathbf{x})) = \int \mathcal{L}(y, g(\mathbf{x})) dP(\mathbf{x}, y)$$

- Empirical (estimated) error:

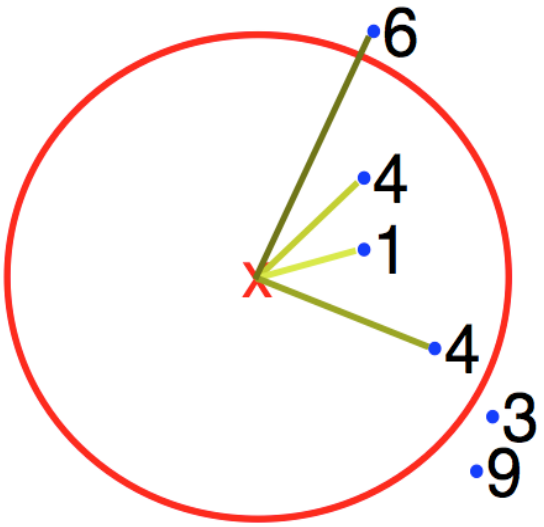
$$L_e(g) = \frac{1}{\ell} \sum_{i=1}^{\ell} \mathcal{L}(y_i, g(\mathbf{x_i}))$$

What is the label for sample x?



k-Nearest Neighbors

k-Nearest Neighbors (k-NN)

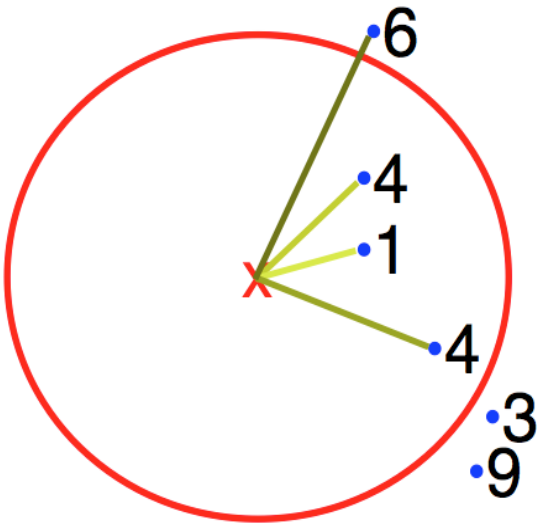


- The k-NN algorithm:

1) For test sample x, we find the k nearest neighbors

2) We label the test sample x using a majority voting on k neighbors

k-Nearest Neighbors (k-NN)



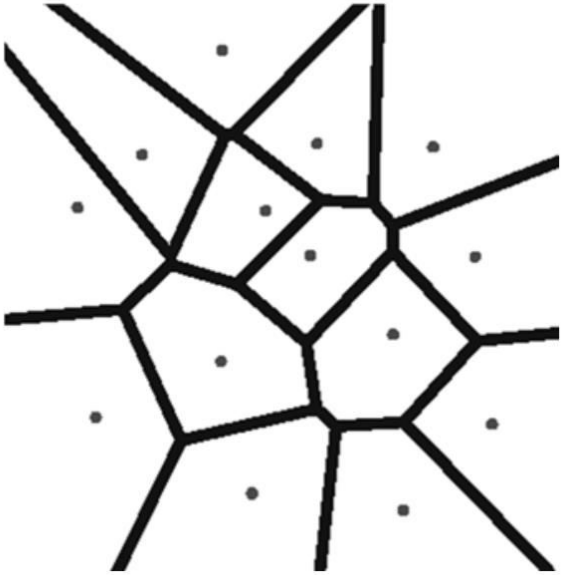
- How do we break ties?

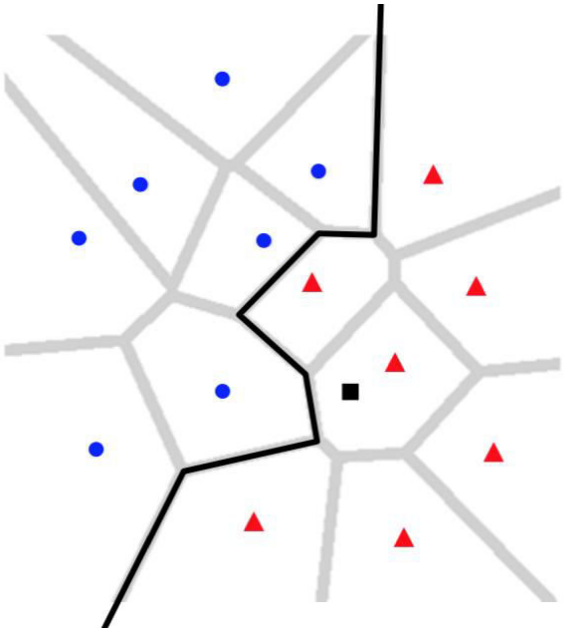
1) Choose a random label from the tied ones

2) Apply 1-NN (no ties possible)

3) Use the distances to the test sample as weights

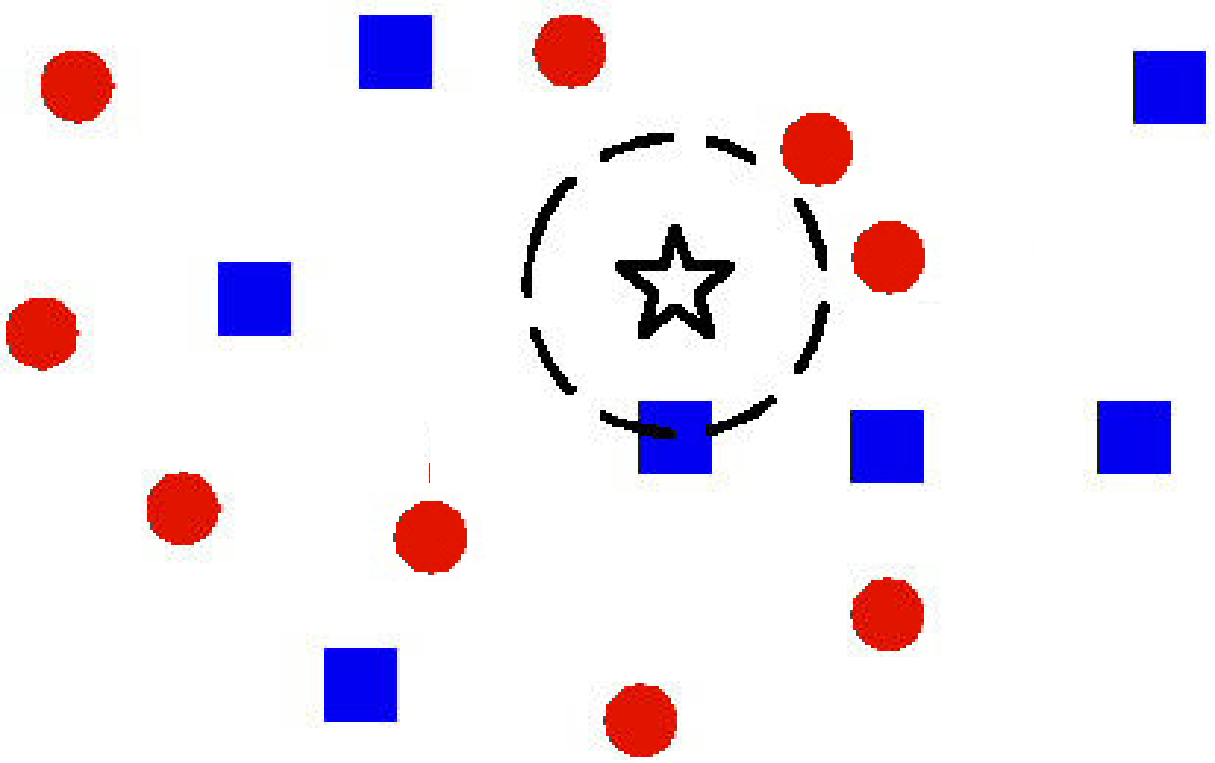
What happens for k = 1?



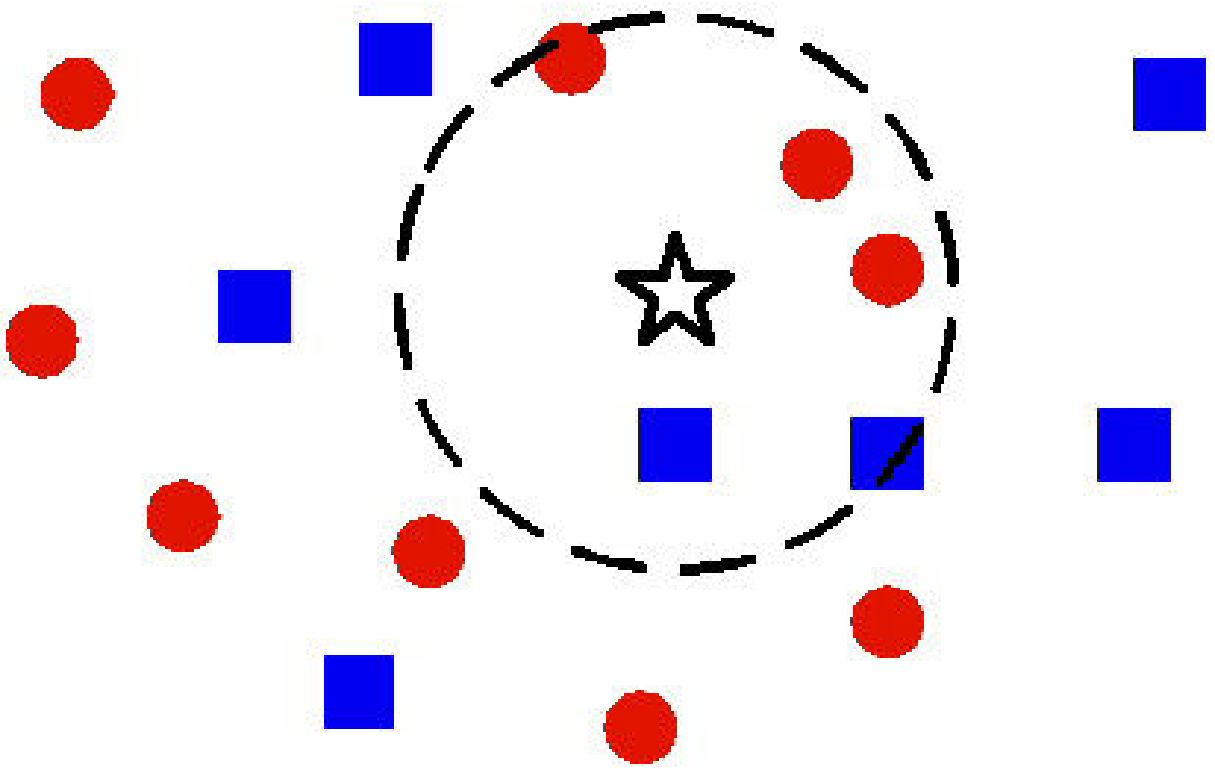


- We obtain a Voronoi diagram:
  - ➢ The space is partitioned into regions
  - ➢ The separating borders pass through areas where the distances between training sample pairs are equal
- The separating borders are nonlinear

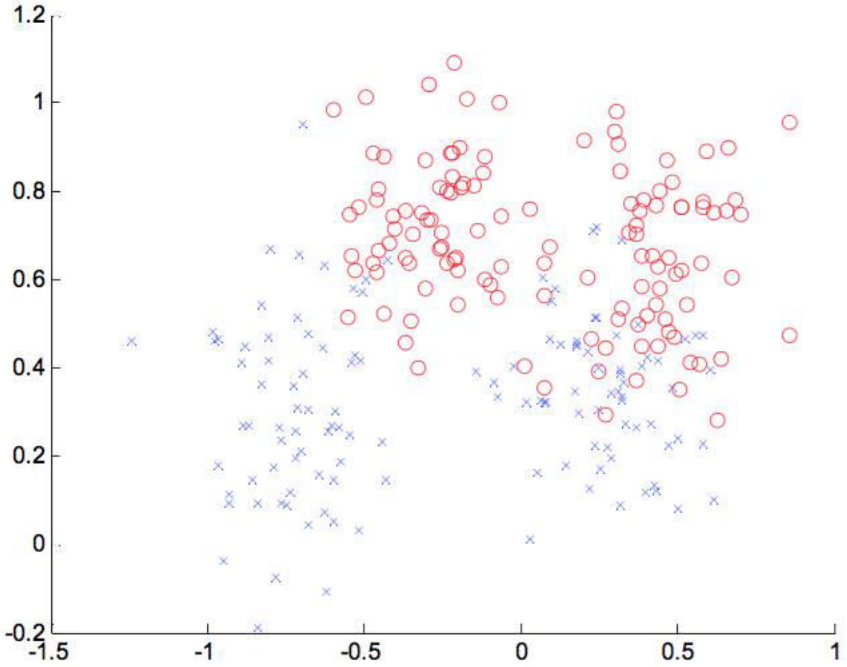
1-NN versus k-NN



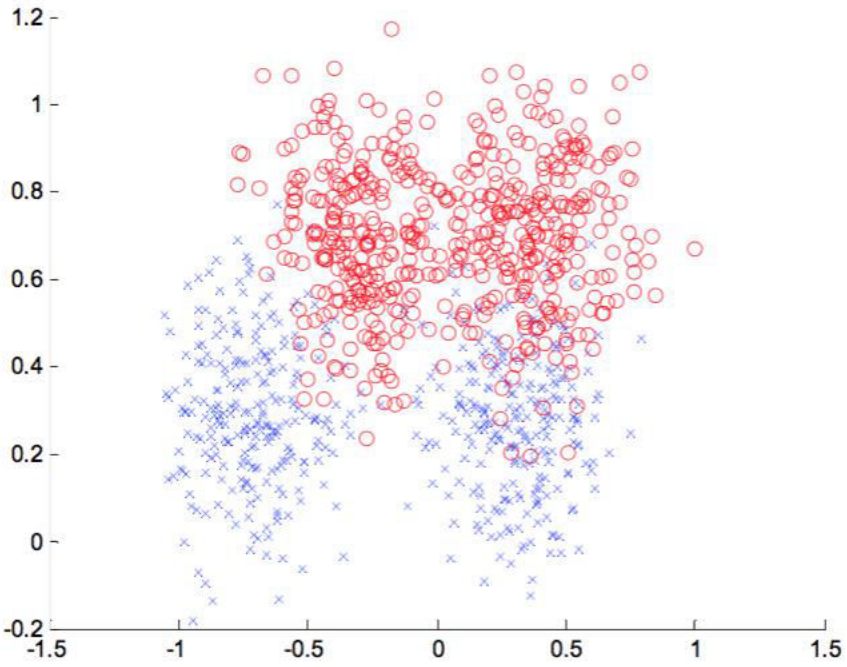
1-NN versus k-NN



The underlying hypothesis of k-NN



Training data

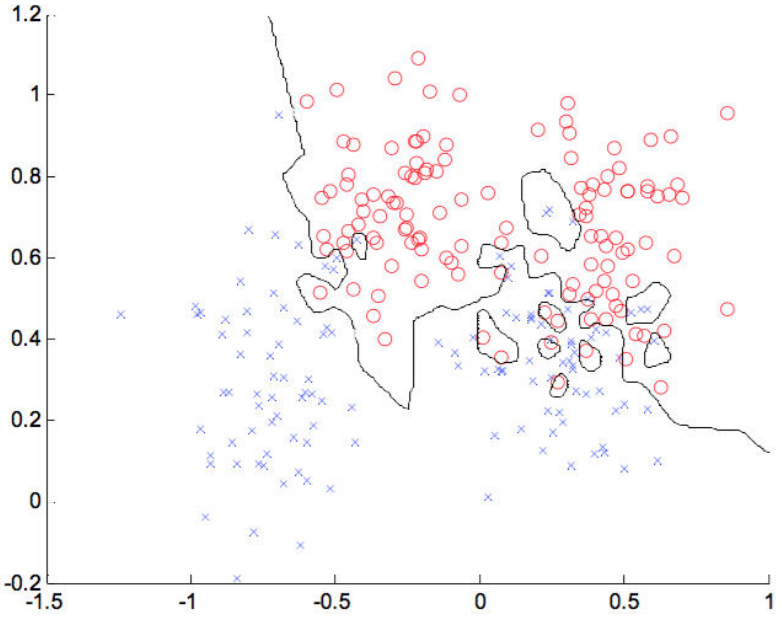


Testing data

- The training data and the test data are sampled from the same distribution
- Becomes unlikely for a representative pattern in the training set to be absent in the test set

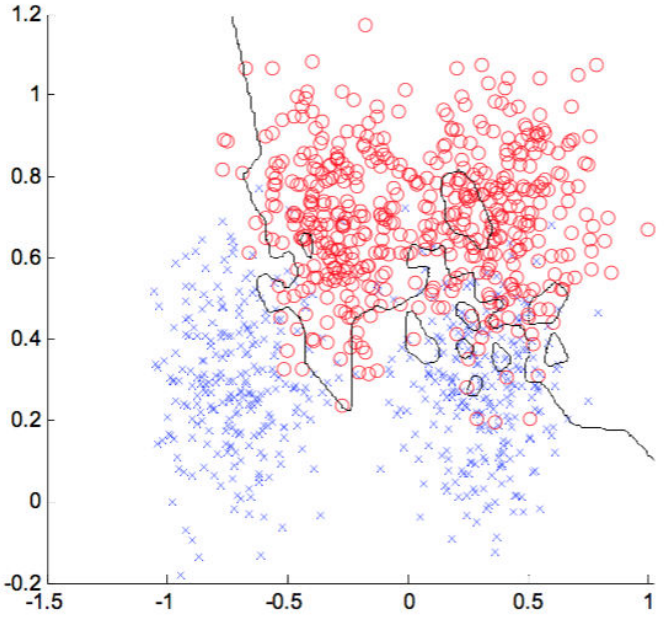
What happens for different values of k?

Training data



error = 0.0

Testing data

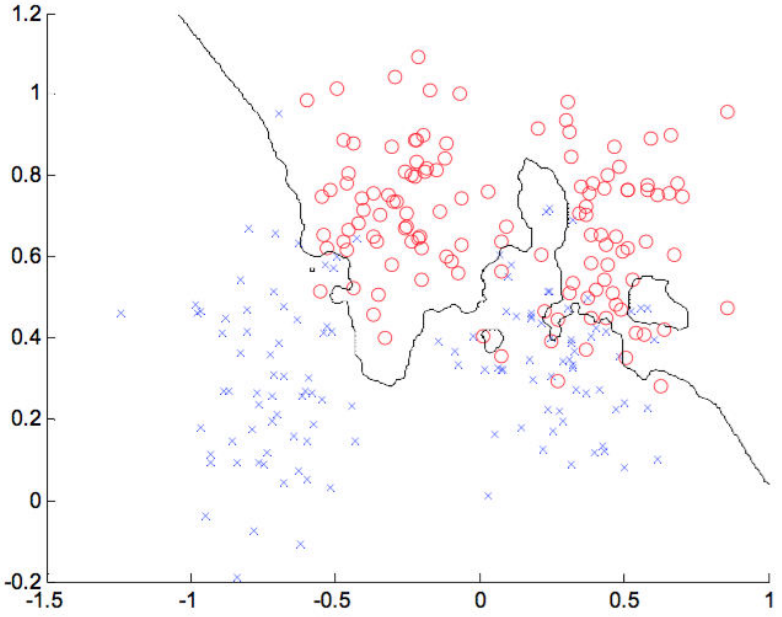


error = 0.15

- k = 1

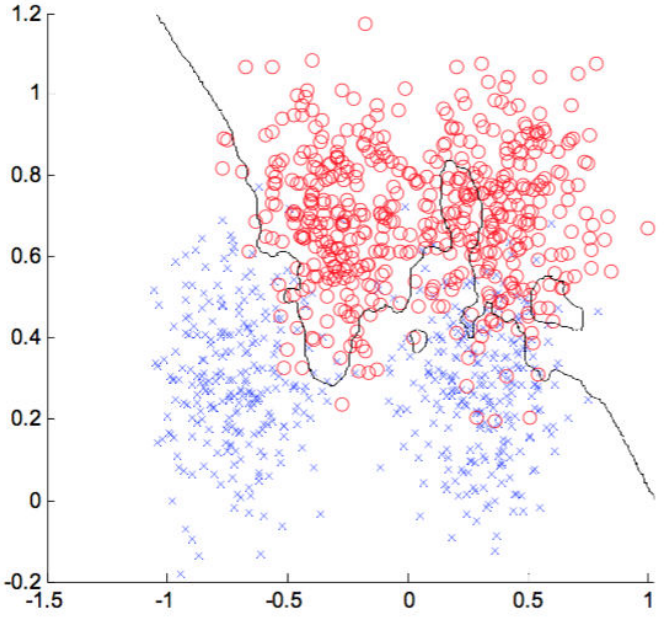
What happens for different values of k?

Training data



error = 0.0760

Testing data

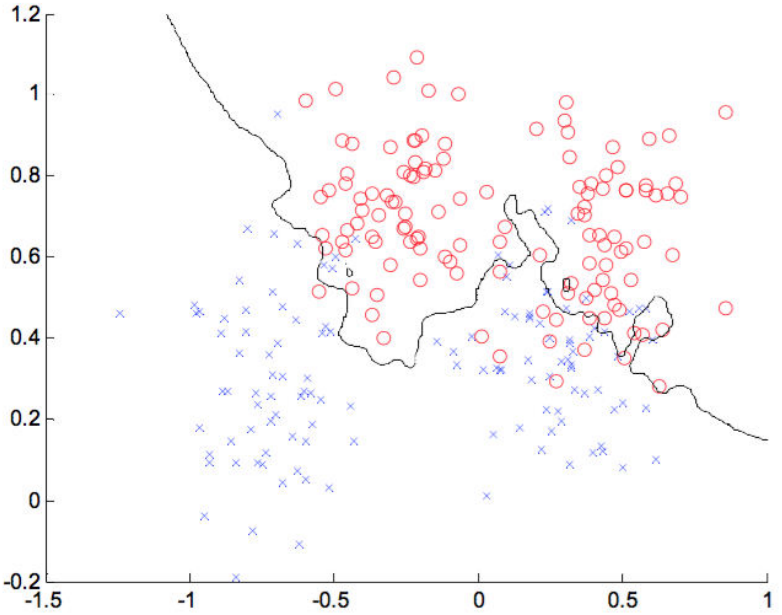


error = 0.1340

- k = 3

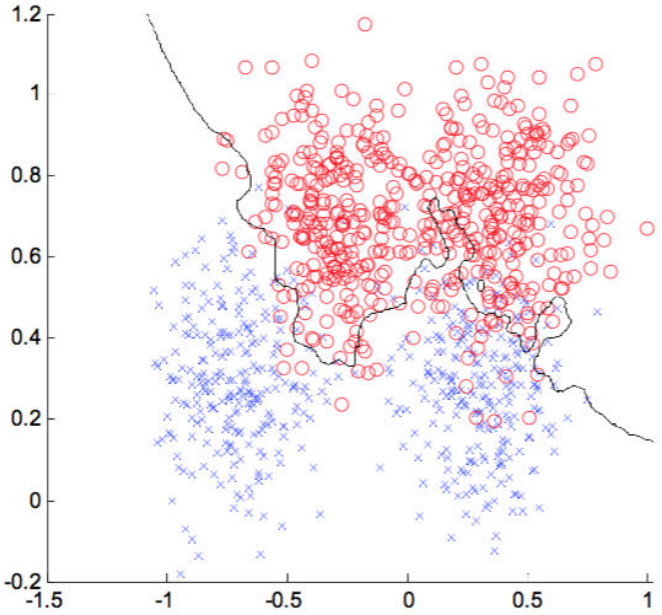
What happens for different values of k?

Training data



error = 0.1320

Testing data

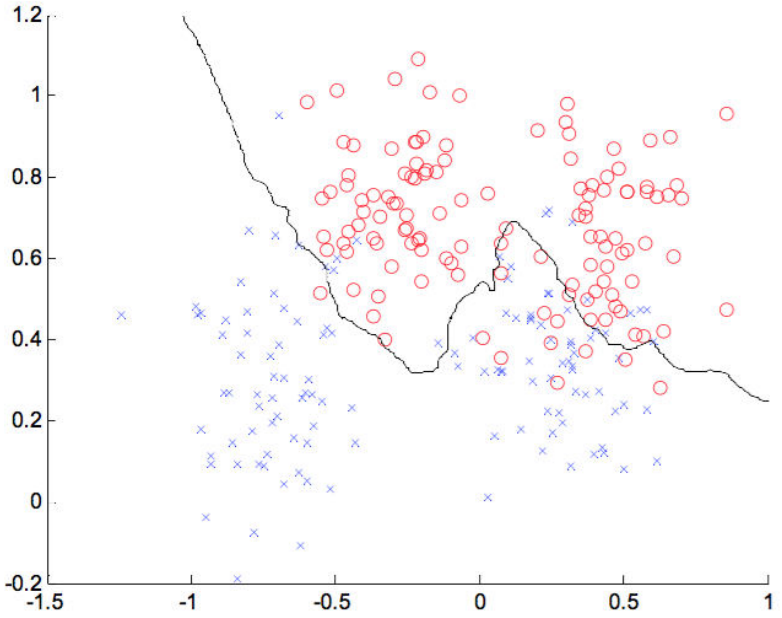


error = 0.1110

- k = 7

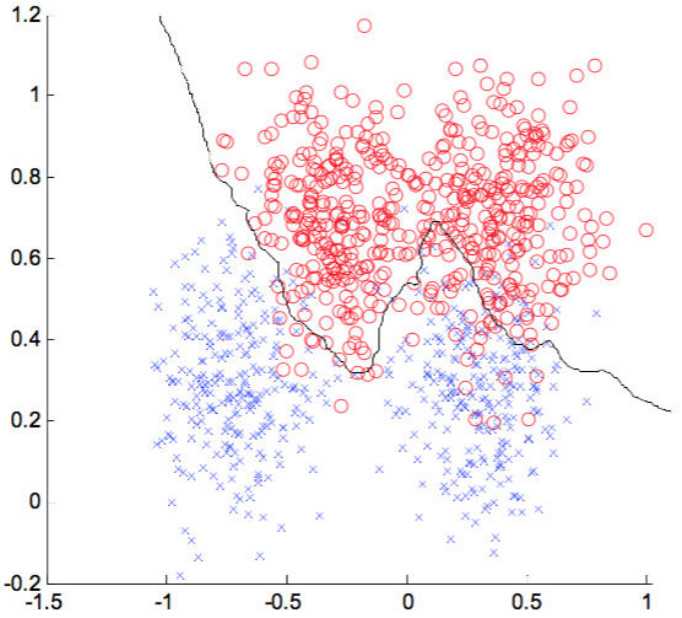
What happens for different values of k?

Training data



error = 0.1120

Testing data



error = 0.0920

- k = 21

What do we need for a memory-based classifier?

- A distance function:
  - **The Euclidean distance**
  - **The Edit (Levenshtein) distance**
  - **The Hamming distance**
- How many neighbors should we consider?
- How do we “train” the model on the examples from the vicinity?

Let's consider a particular 1-NN

- A distance function:
- **E.g., the Euclidean distance**

- How many neighbors should we consider?
- **1**

- How do we "train" the model on the examples from the vicinity?
- **We just predict the label of the nearest neighbor**

The Euclidean distance (L_2)

- For the vectors $x = (5, 1,3,0)$ and $y = (2,1,4,1)$, we have:

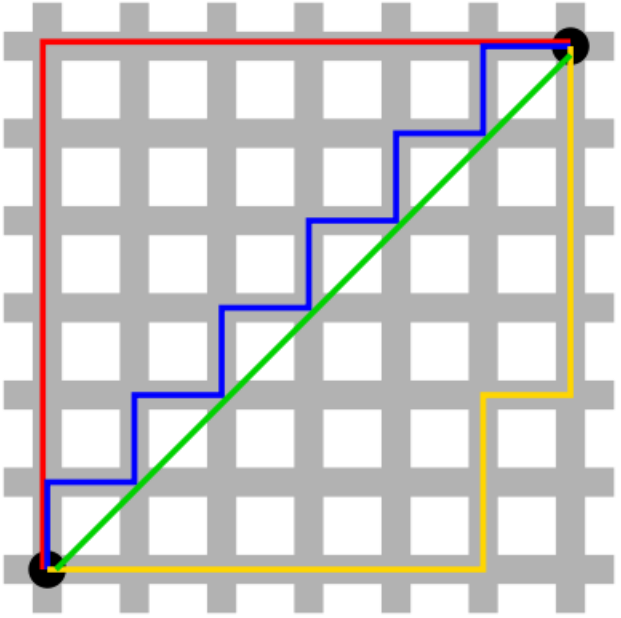
$$d_{L_2}(x, y) = \sqrt{(x_1 - y_1)^2 + \cdots + (x_n - y_n)^2}$$

$$= \sqrt{(5-2)^2 + (1-1)^2 + (3-4)^2 + (0-1)^2}$$

$$= \sqrt{9 + 1 + 1} = \sqrt{11}$$

$$\cong 3.32$$

The Manhattan distance (L_1)



- For the vectors $x = (5, 1,3,0)$ and $y = (2,1,4,1)$, we have:

$$d_{L_1}(x, y) = |x_1 - y_1| + \cdots + |x_n - y_n|$$

$$= |5 - 2| + |1 - 1| + |3 - 4| + |0 - 1|$$

$$= 3 + 1 + 1 = 5$$

The Minkowski distance (L_p)

- For the vectors $x = (x_1, \dots, x_n)$ and $y = (y_1, \dots, y_n)$, we have:

$$d_{L_p}(x, y) = \sqrt[p]{|x_1 - y_1|^p + \cdots + |x_n - y_n|^p}$$

- The Minkowski distance is a generalization for the Euclidean distance ($p = 2$) and the Manhattan distance ($p = 1$)
- If $p < 1$, then $d_{L_{p<1}}$ is no longer a distance. The triangle inequality is violated for $x = (0,0)$, $y = (1,1)$ and $z = (0,1)$:

$$d_{L_{p<1}}(x, y) > d_{L_{p<1}}(x, z) + d_{L_{p<1}}(z, y)$$

The Hamming distance

- Useful, for instance, when the samples are represented by categorical features or when the samples are DNA sequences
- For the vectors $x = (A, G, T, C)$ and $y = (G, G, T, A)$, we have:

$$d_{Hamming}(x, y) = 1 + 0 + 0 + 1 = 2$$

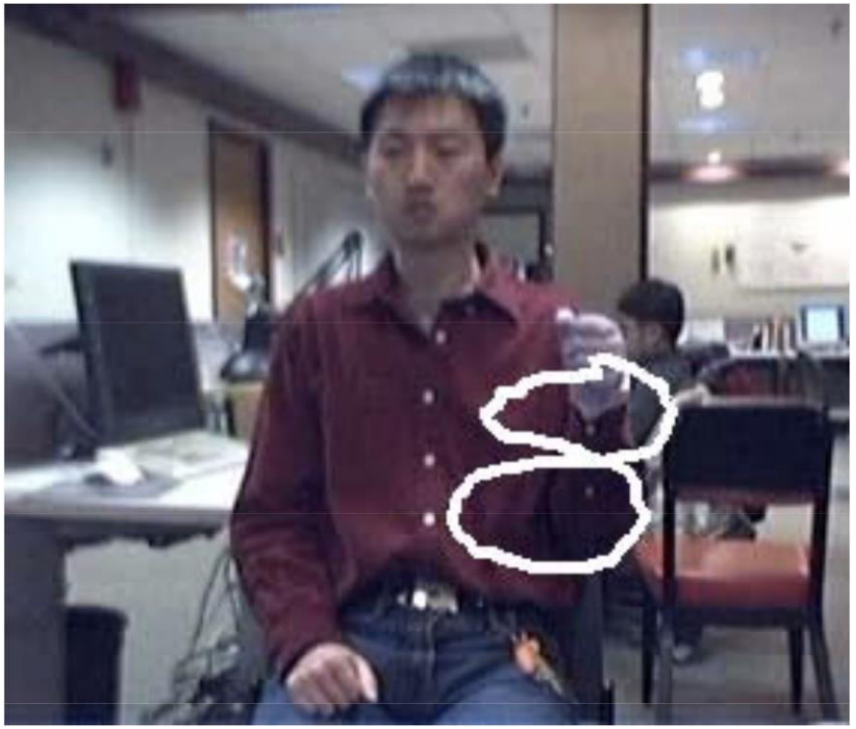
- We are counting how many features (components) are different among the two vectors

The Edit (Levenshtein) distance

- Useful, for instance, when the samples are strings (text documents, DNA sequences) or temporal sequences (videos)
- The distance is given by the number of changes (insert, delete, replace) necessary to transform one object into the other
- For video sequences, we use Dynamic Time Warping (DTW)

Application: Gesture recognition

- What gesture corresponds to the motion performed by the user?



Let’s consider 10 gesture classes

Gesture recognition problem

- We have to recognize 10 simple gestures performed by a user
- Each gesture corresponds to a number from 0 to 9

- Only the trajectory of the hand matters, not the handshape / fingers pose:
  - ➢ This is just a choice we make for this example application
  - ➢ Many systems, e.g. sign language, need to use handshape as well

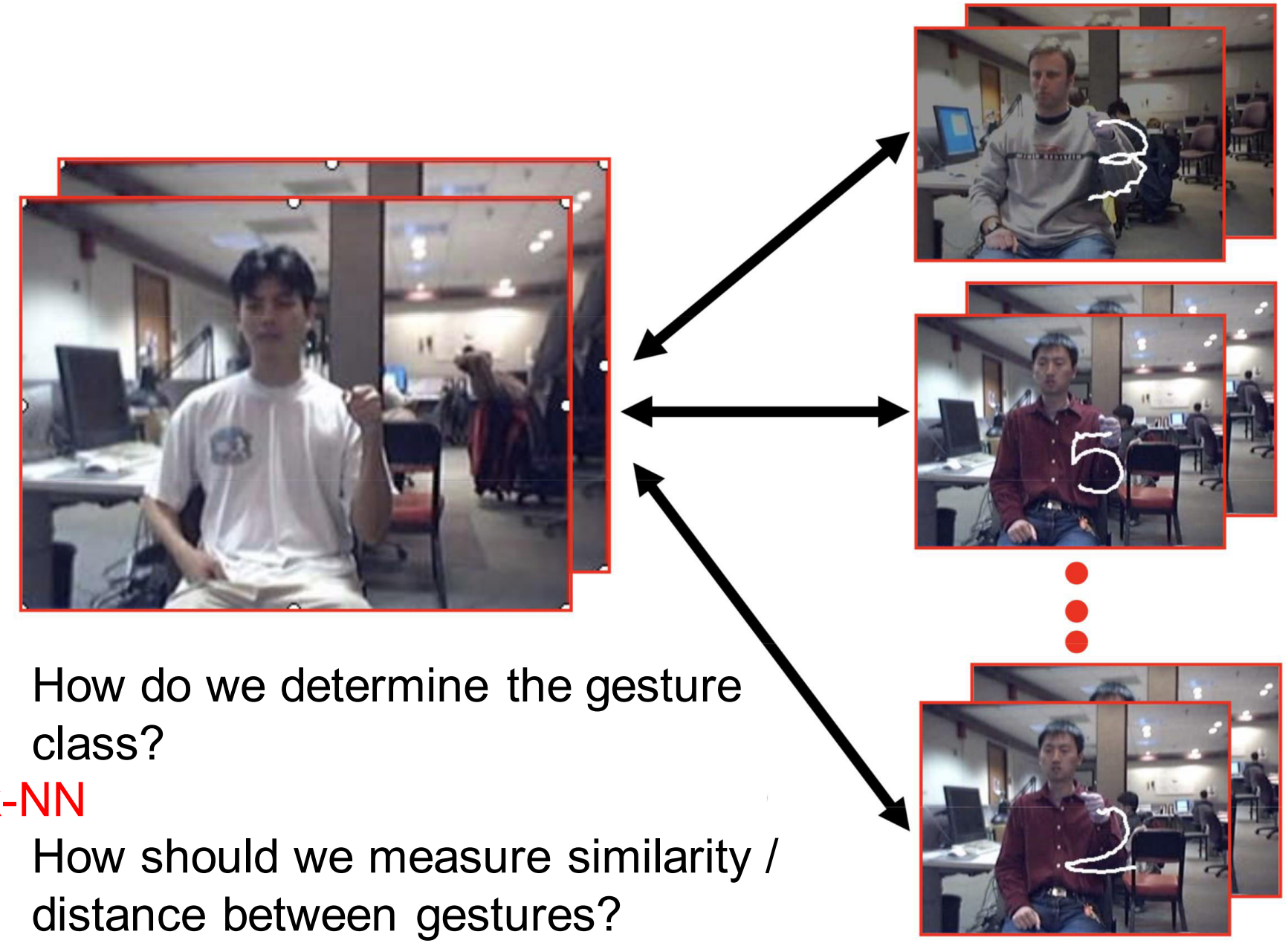
Decomposing gesture recognition

We need modules for:

- Computing how the person moved
  - Person detection / tracking
  - Hand detection / tracking
  - Handshape recognition?

- Recognizing what the motion means
  - Motion estimation and recognition are quite different tasks
  - When we see someone using sign language, we know how they move, but not what the motion means

Gesture recognition

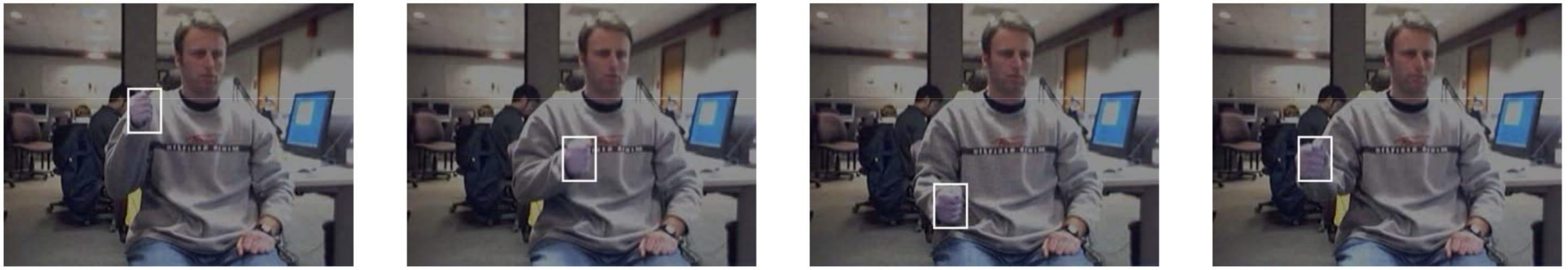


- How do we determine the gesture class?

k-NN

- How should we measure similarity / distance between gestures?

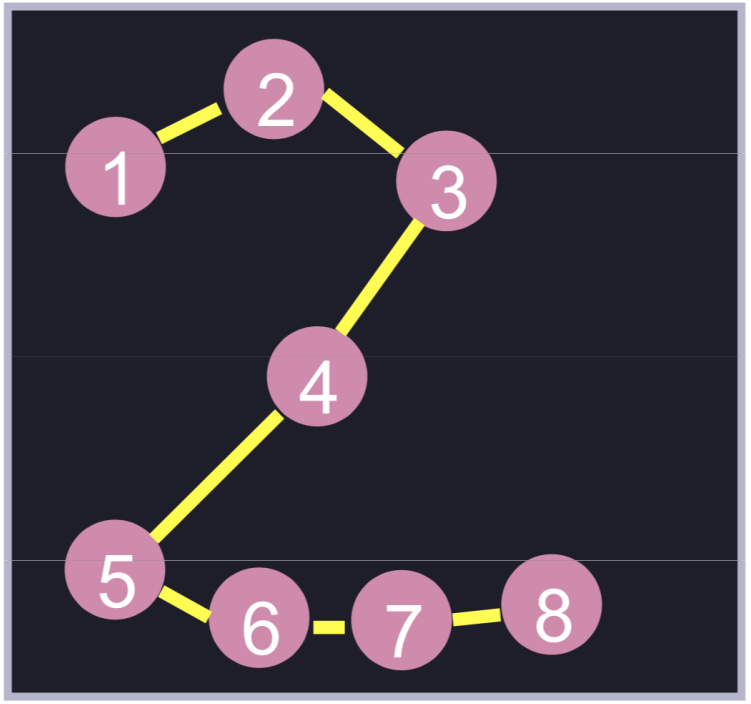
If hand location is known

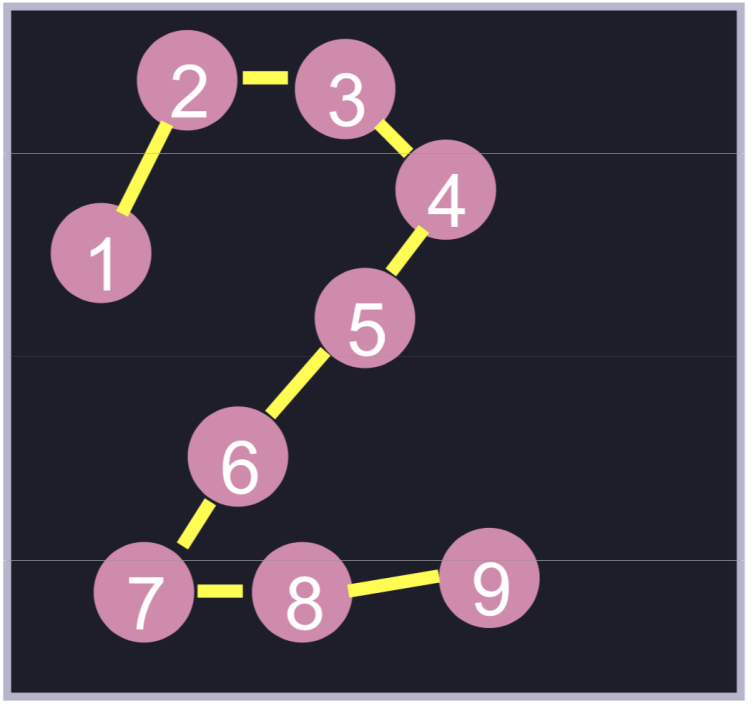


- Assumption: hand location is known in all frames of the database gestures
- The training data can be annotated offline using manual annotation / colored gloves / sensors
- For the test data, we need a hand detector

(we do not cover this part)

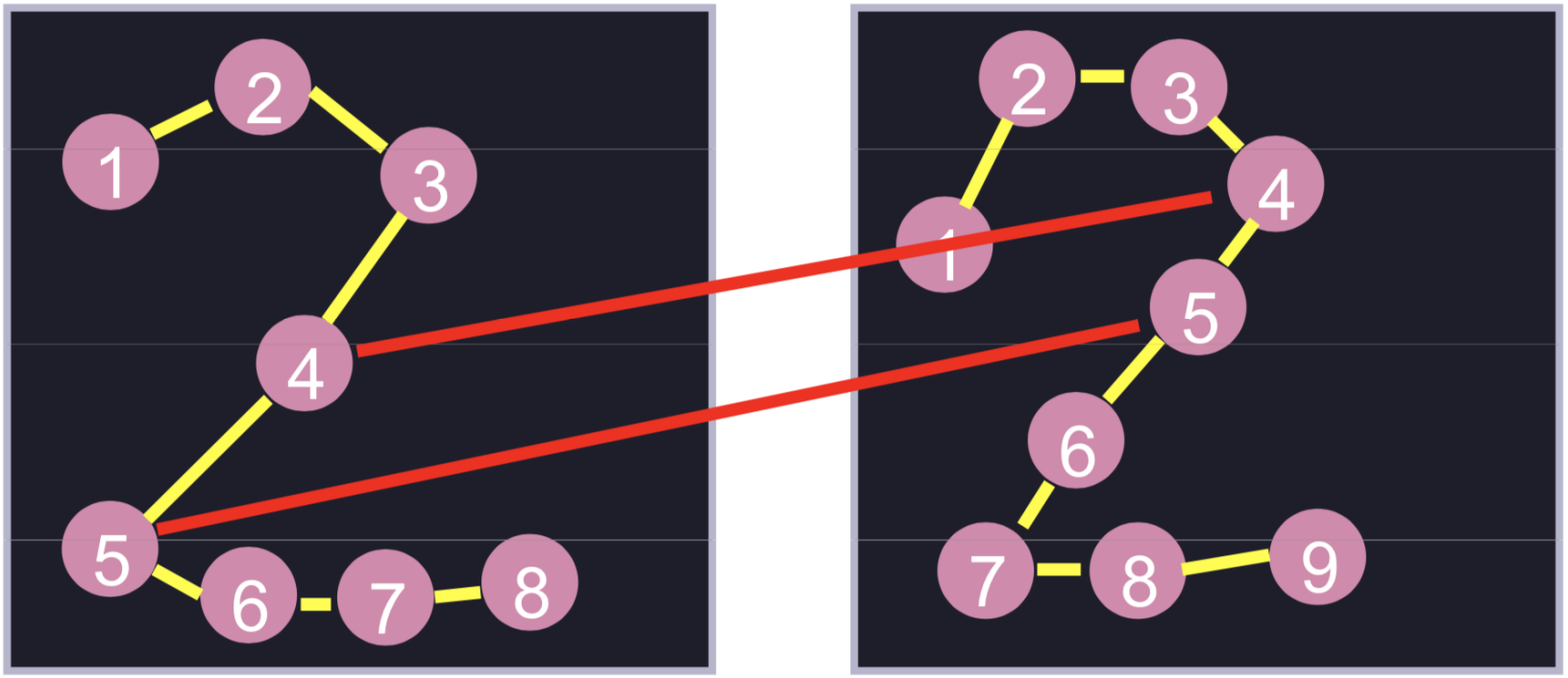
Comparing trajectories





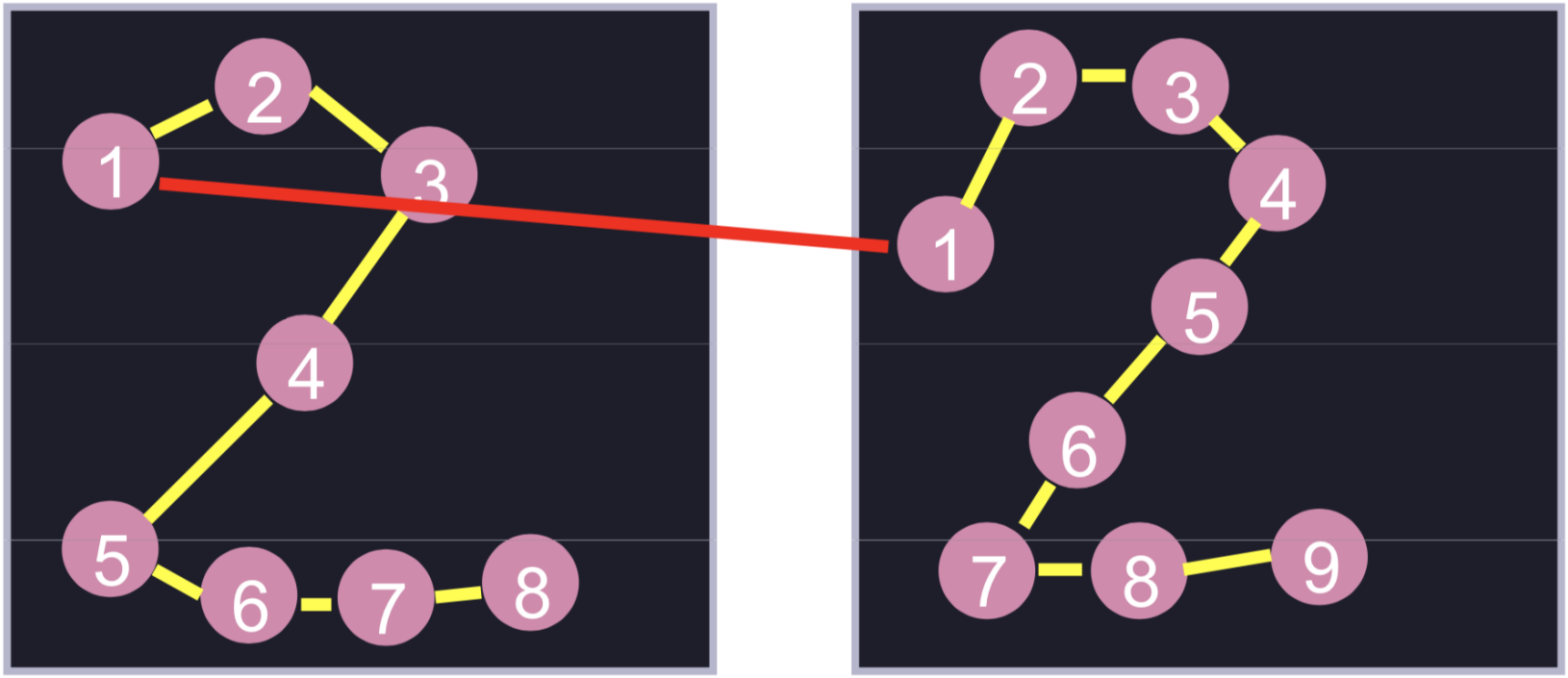
- We can make a trajectory based on the location of the hand at each frame
- How do we compare trajectories?

Matching trajectories



- Comparing i-th frame to i-th frame is problematic
- What do we do with frame 9 from the right?

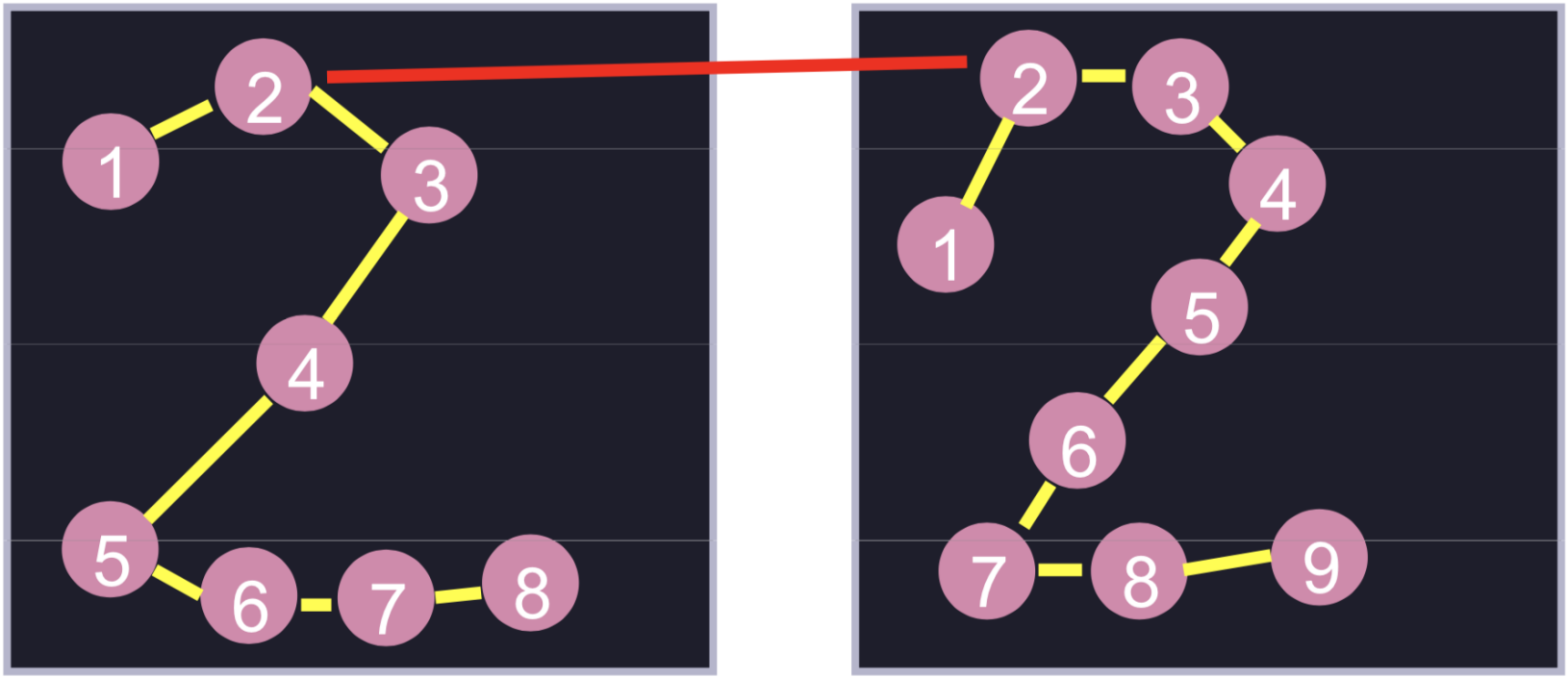
Matching trajectories



- We can align them:

((1, 1)

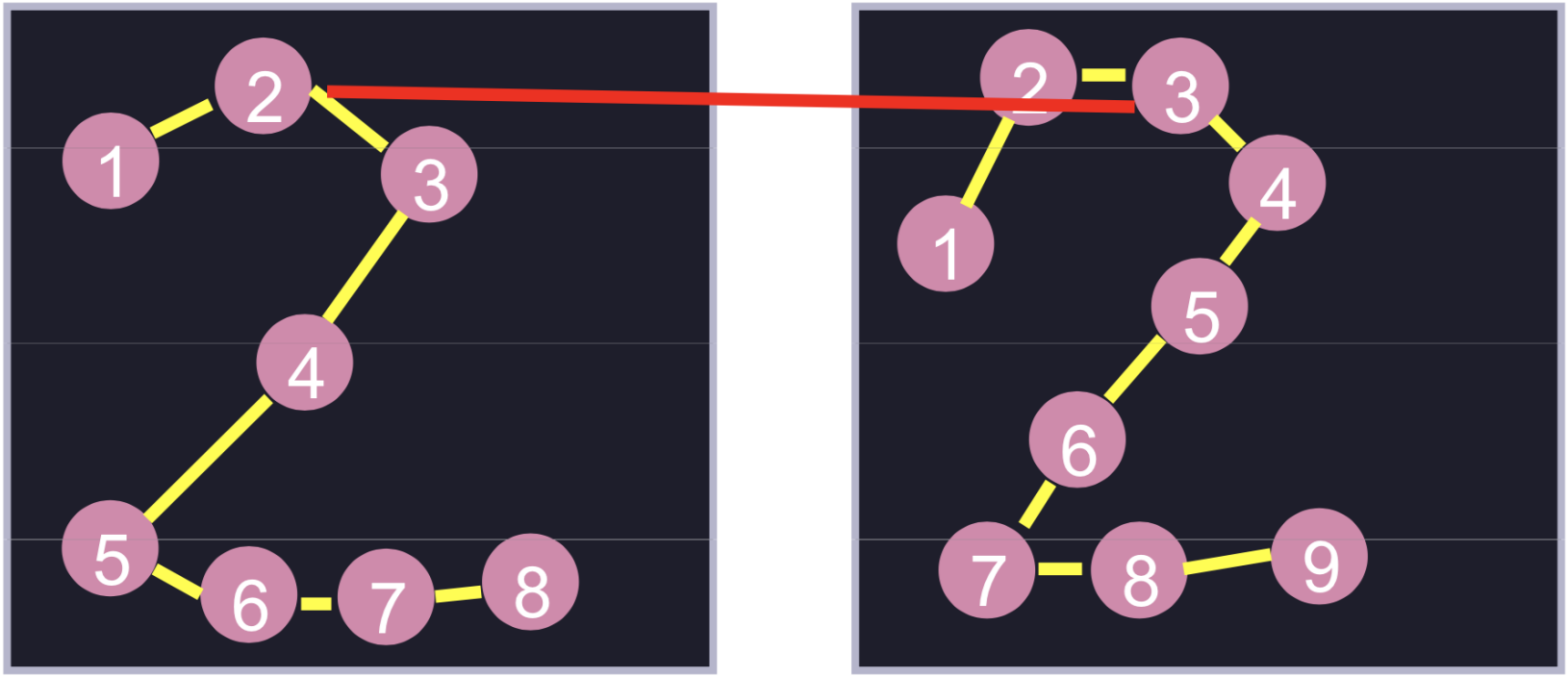
Matching trajectories



- We can align them:

((1, 1), (2, 2)

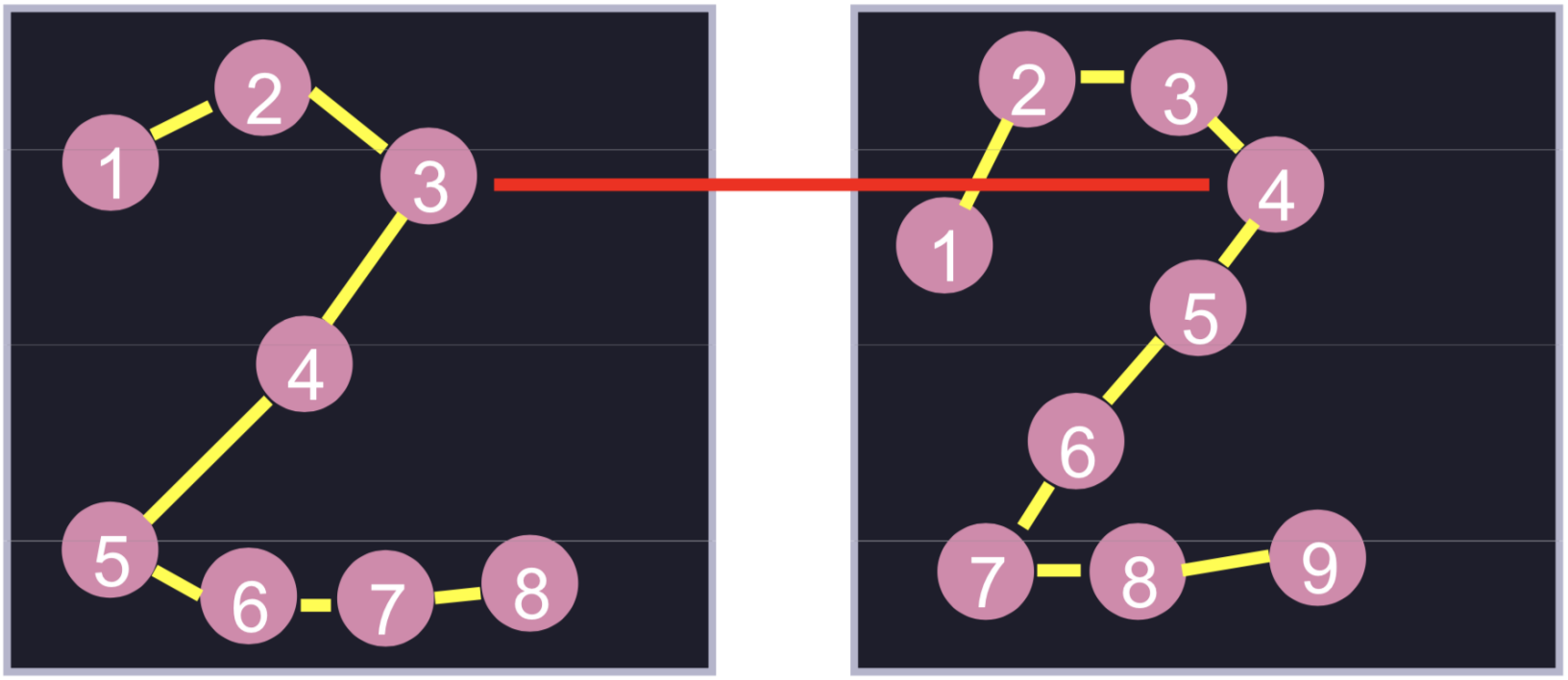
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3)

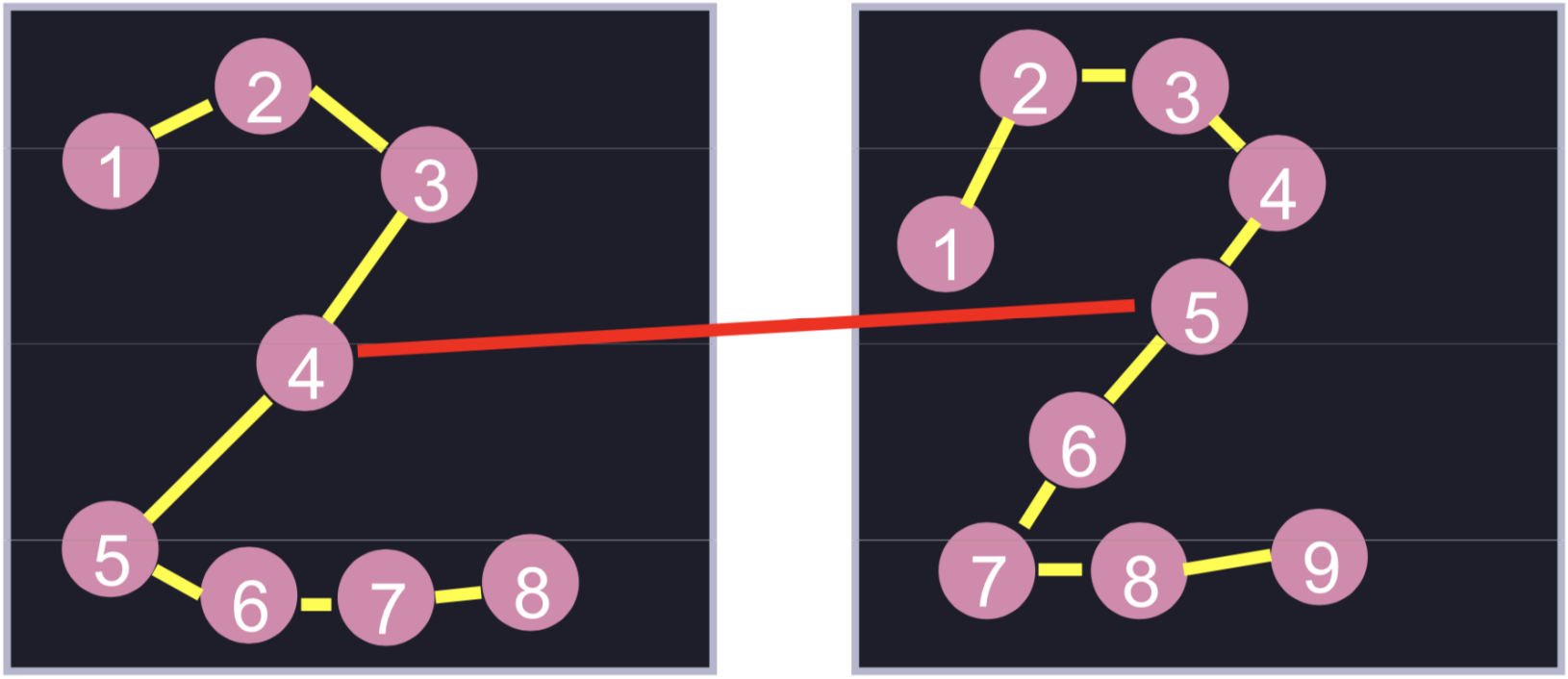
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4)

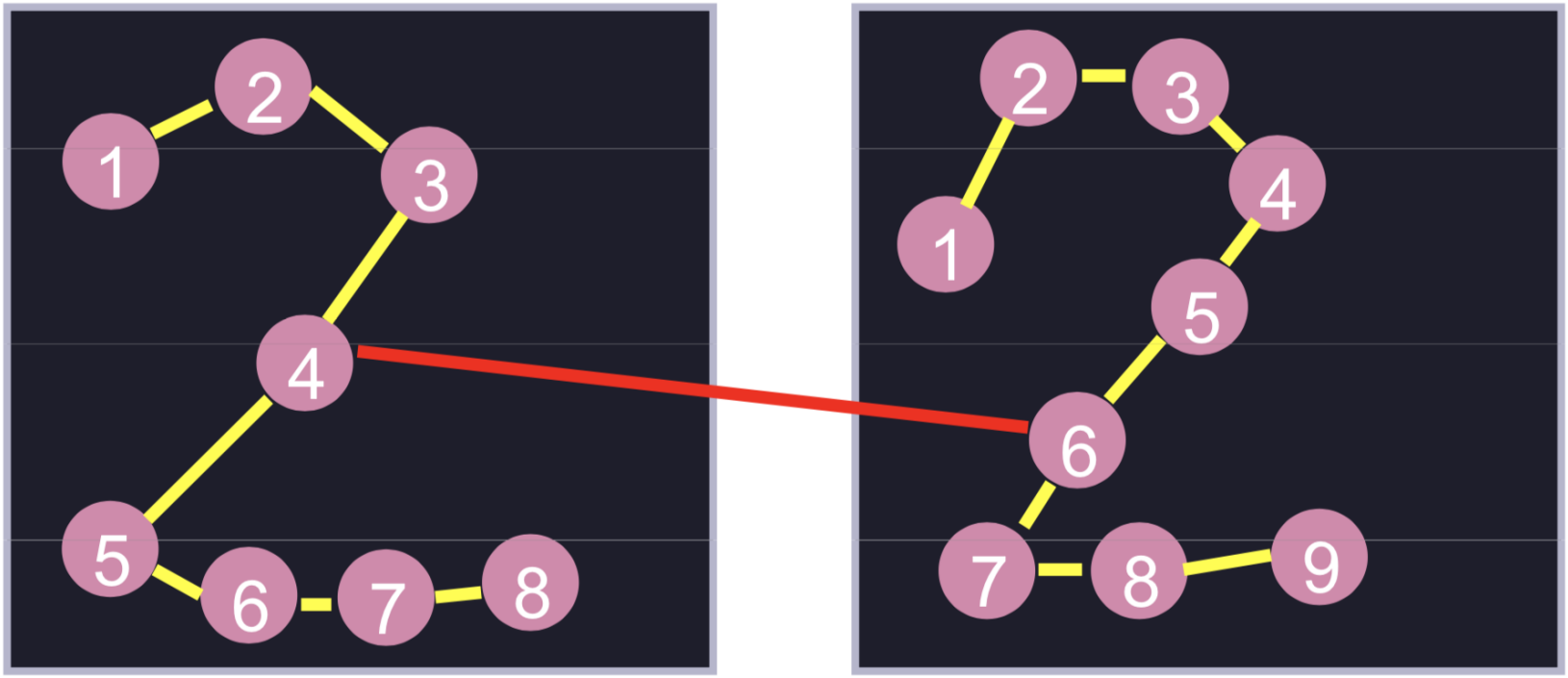
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5)

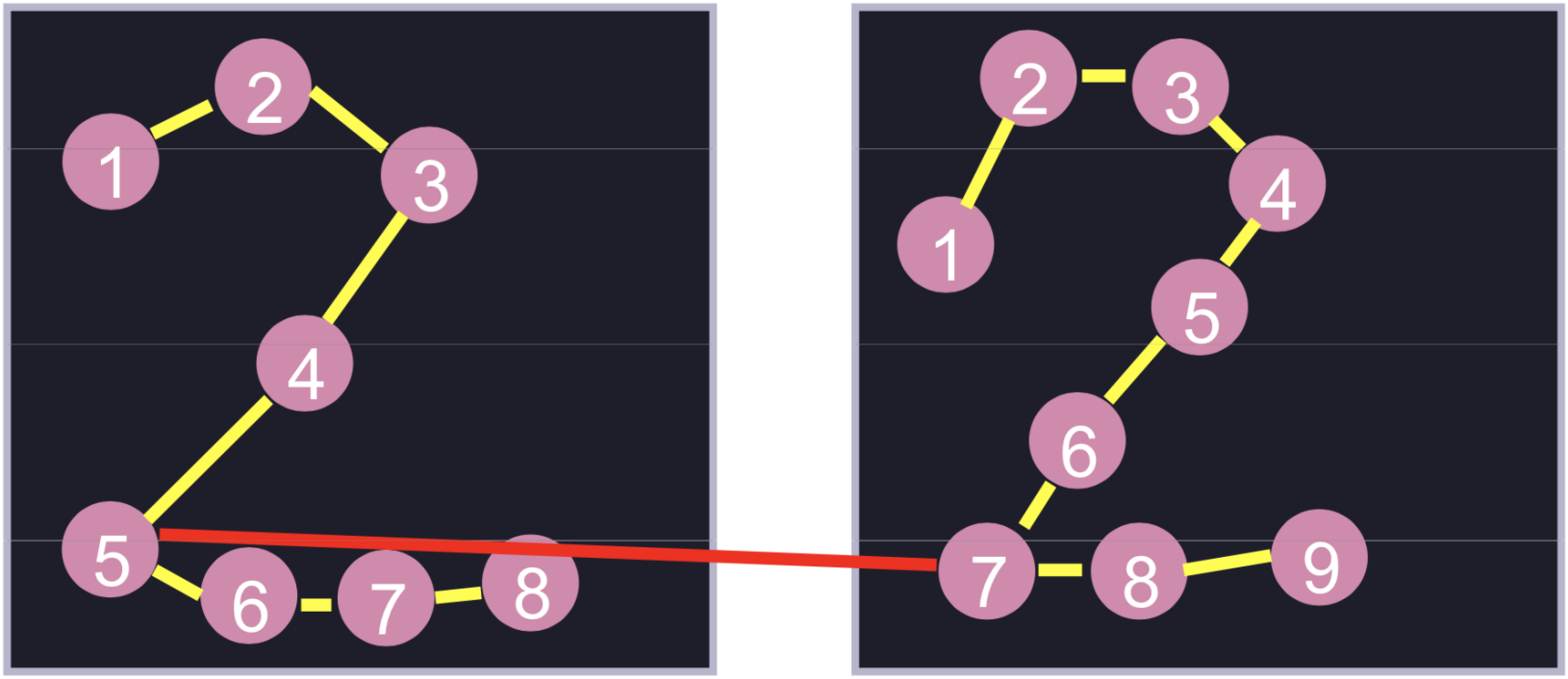
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6)

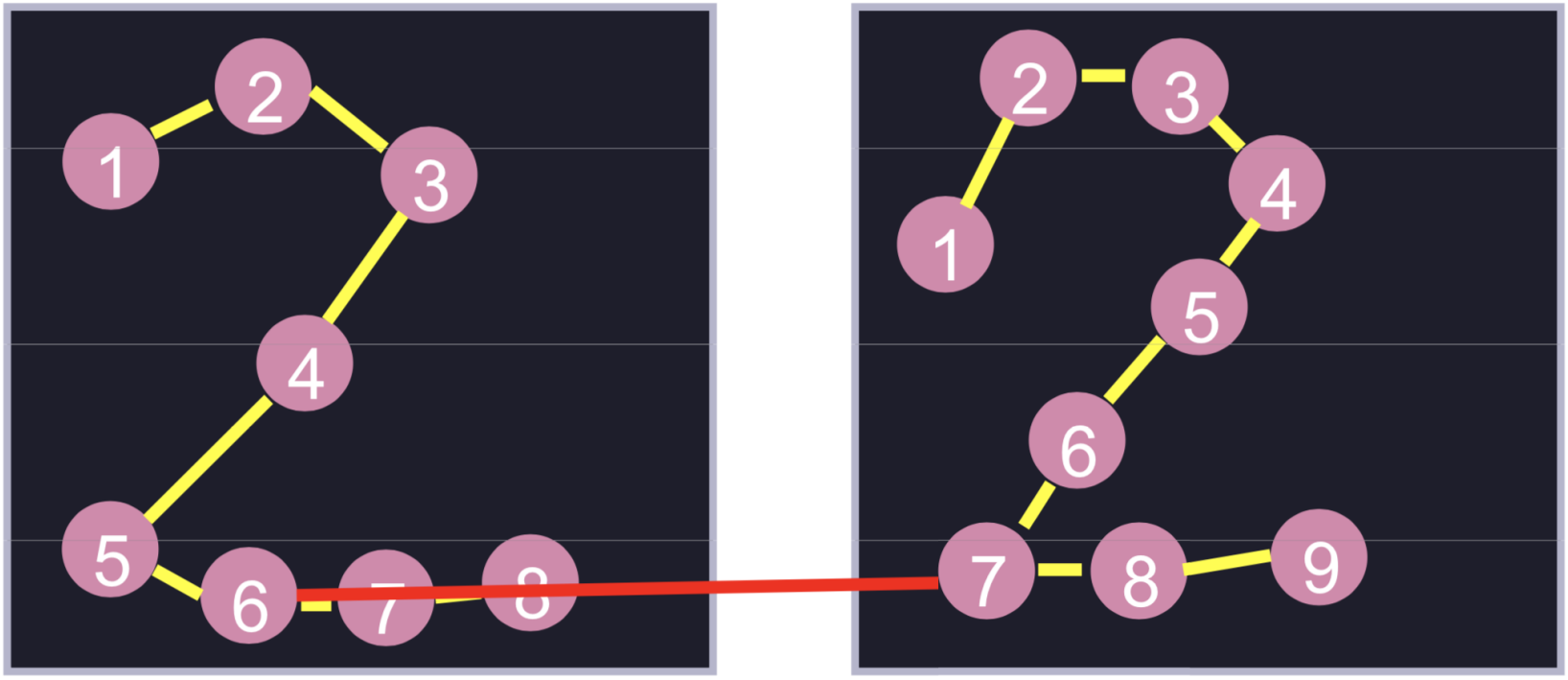
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7)

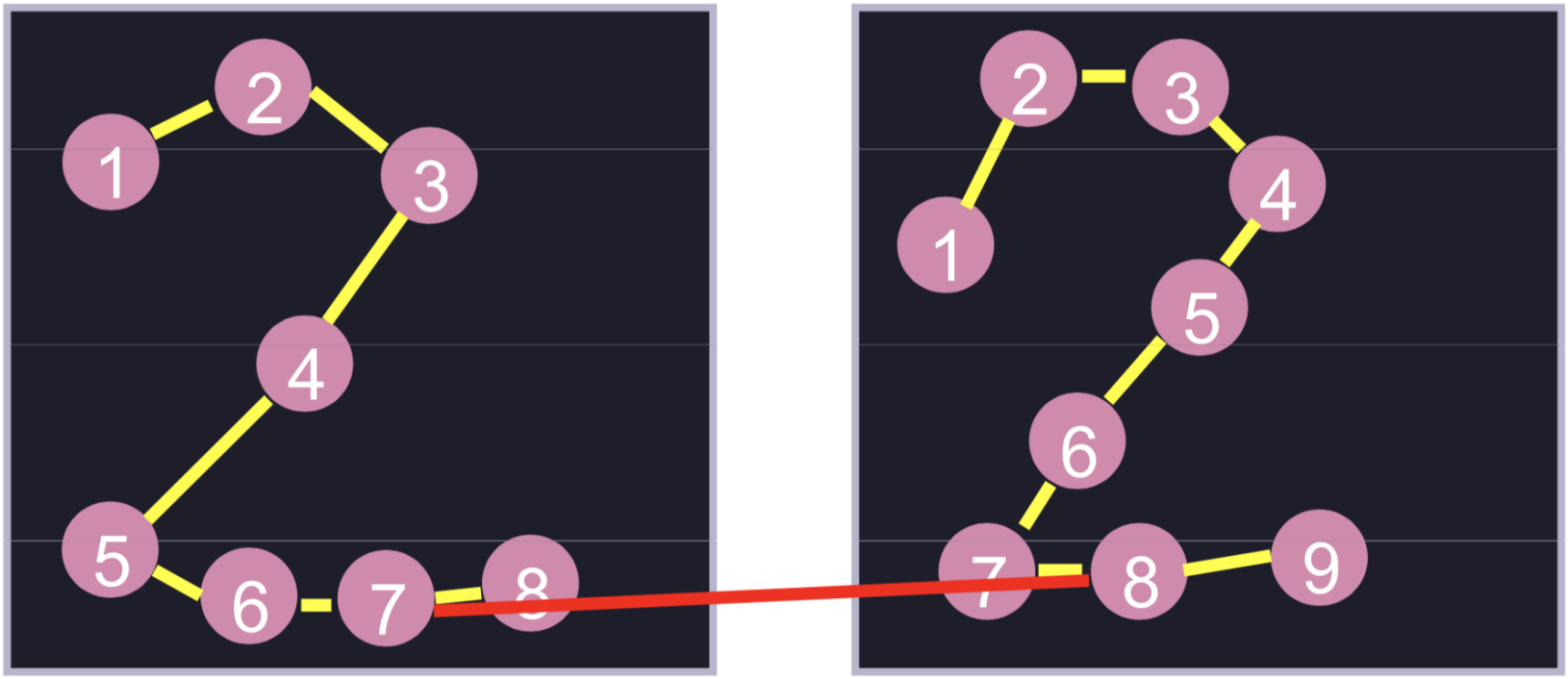
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7)

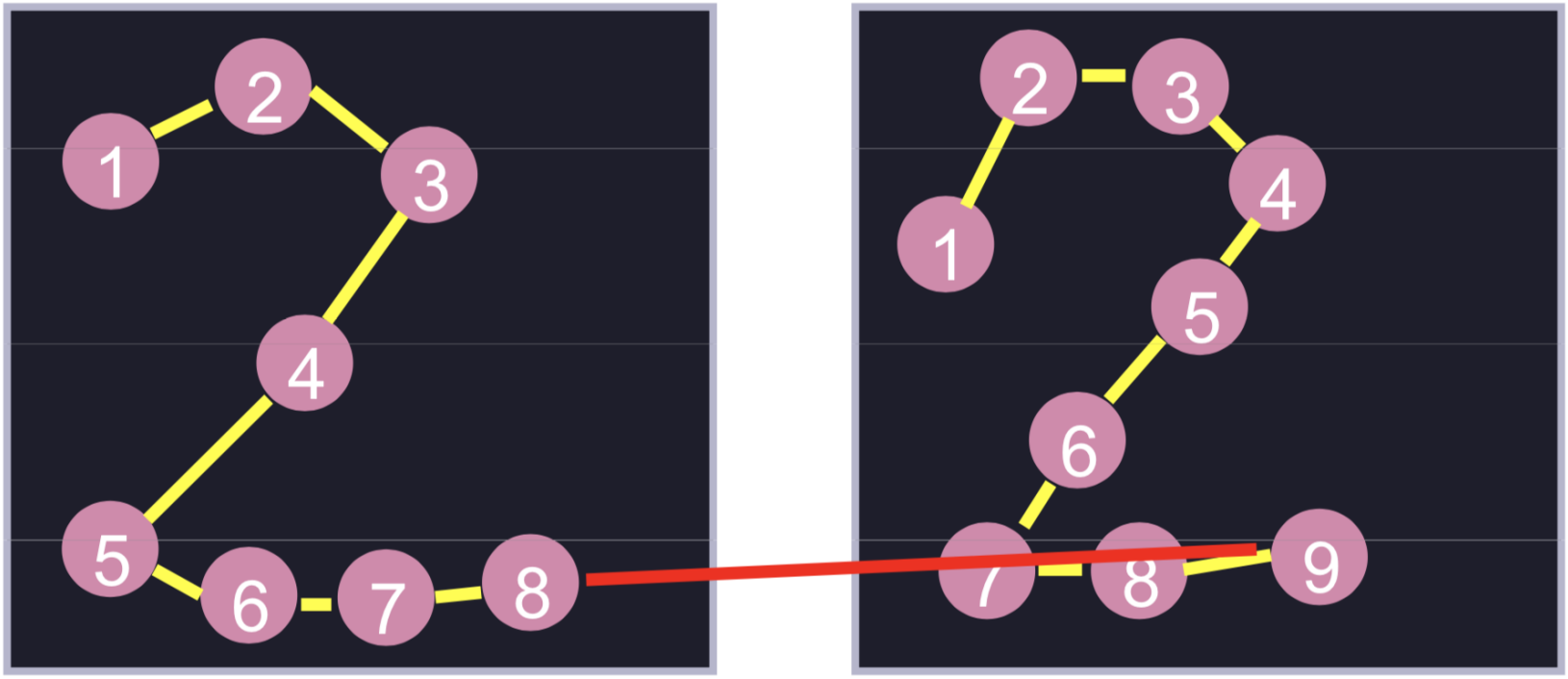
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8)

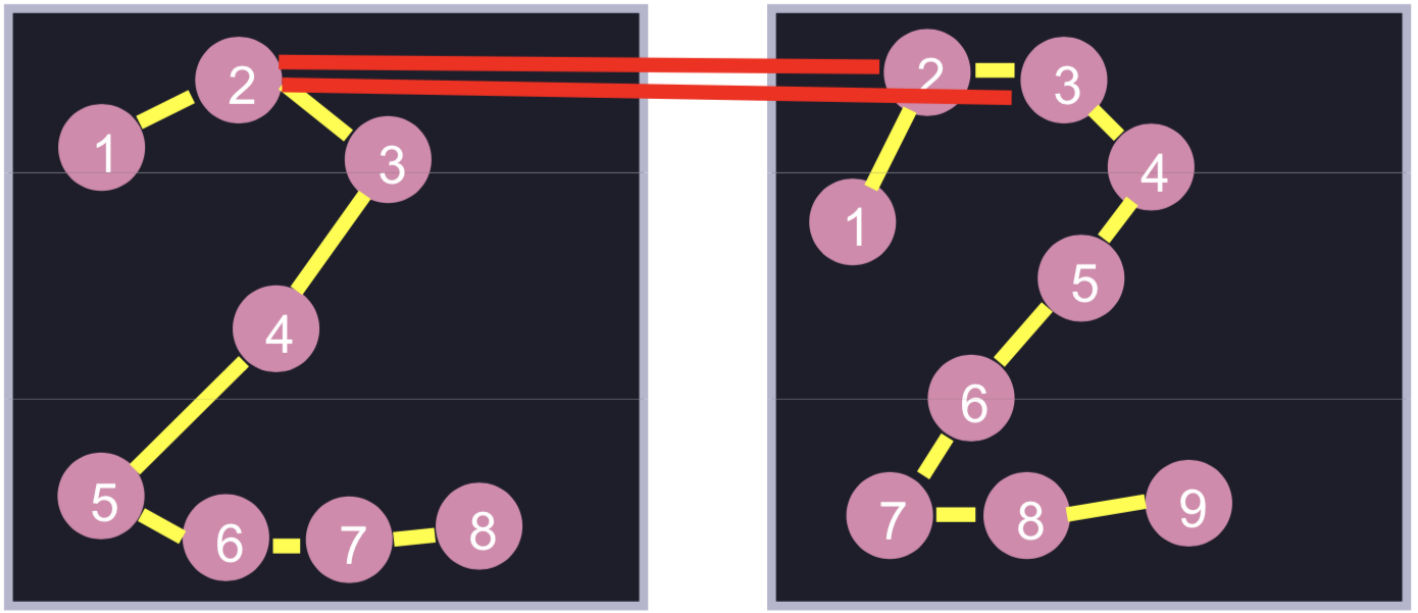
Matching trajectories



- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

Matching trajectories



$M = (M_1, M_2, \ldots, M_8)$.

$Q = (Q_1, Q_2, \ldots, Q_9)$.

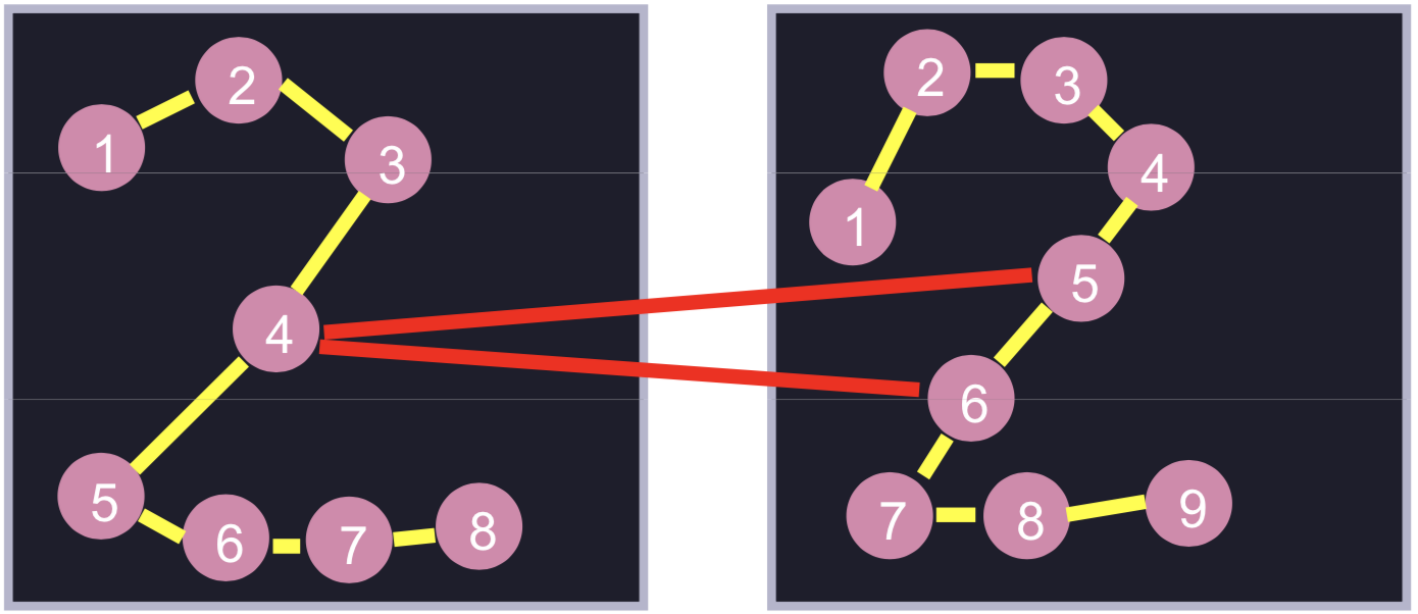
- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- Can be many-to-many:

M_2 is matched with Q_2 and Q_3

Matching trajectories



$M = (M_1, M_2, \ldots, M_8)$.

$Q = (Q_1, Q_2, \ldots, Q_9)$.

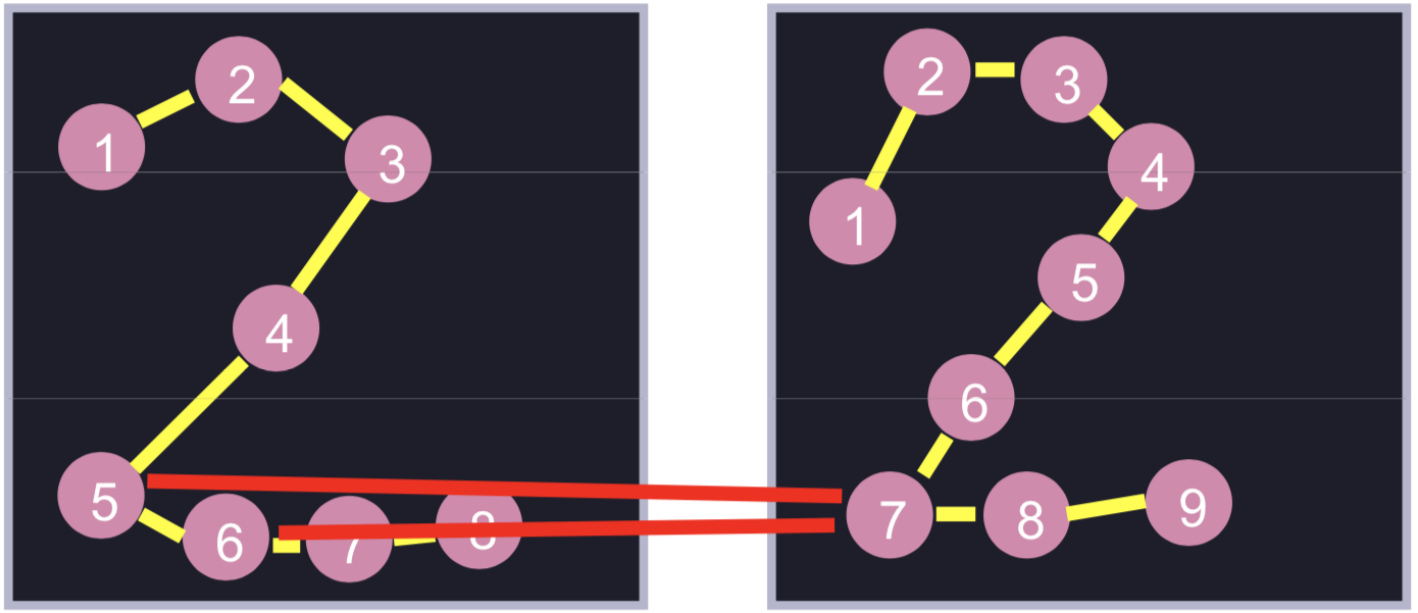
- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- Can be many-to-many:

M_4 is matched with Q_5 and Q_6

Matching trajectories



$M = (M_1, M_2, \ldots, M_8)$.

$Q = (Q_1, Q_2, \ldots, Q_9)$.

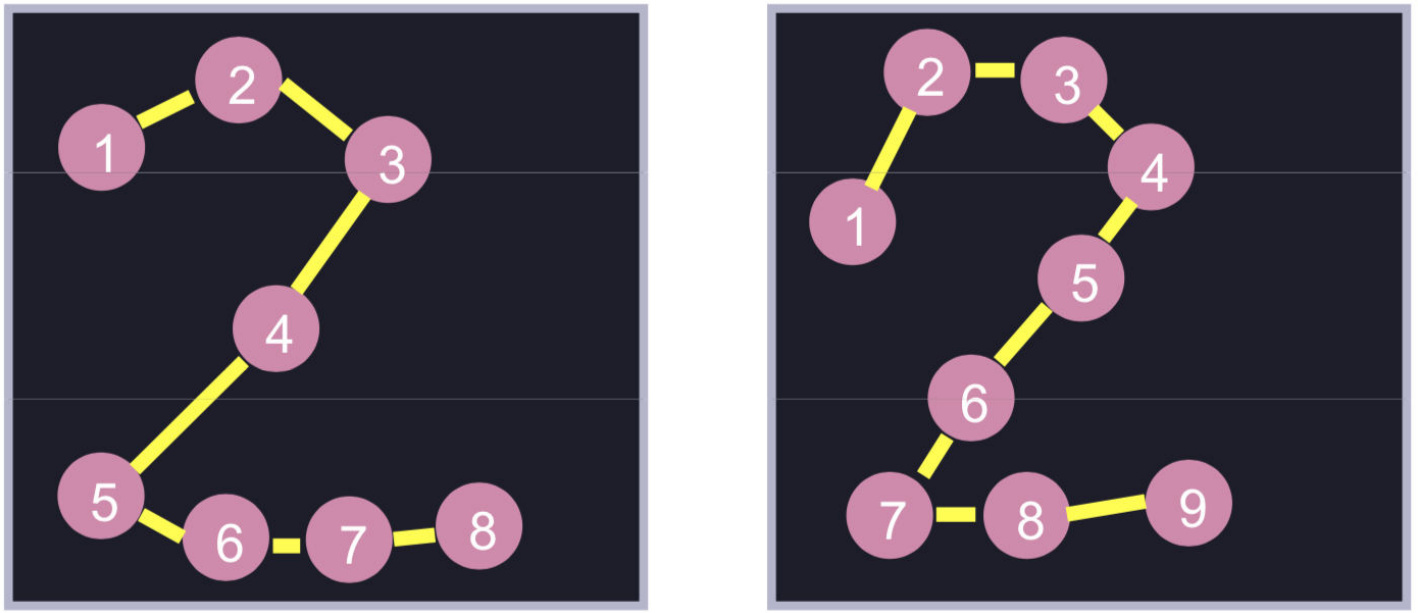
- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- Can be many-to-many:

M_5 and M_6 are matched with Q_7

Matching trajectories

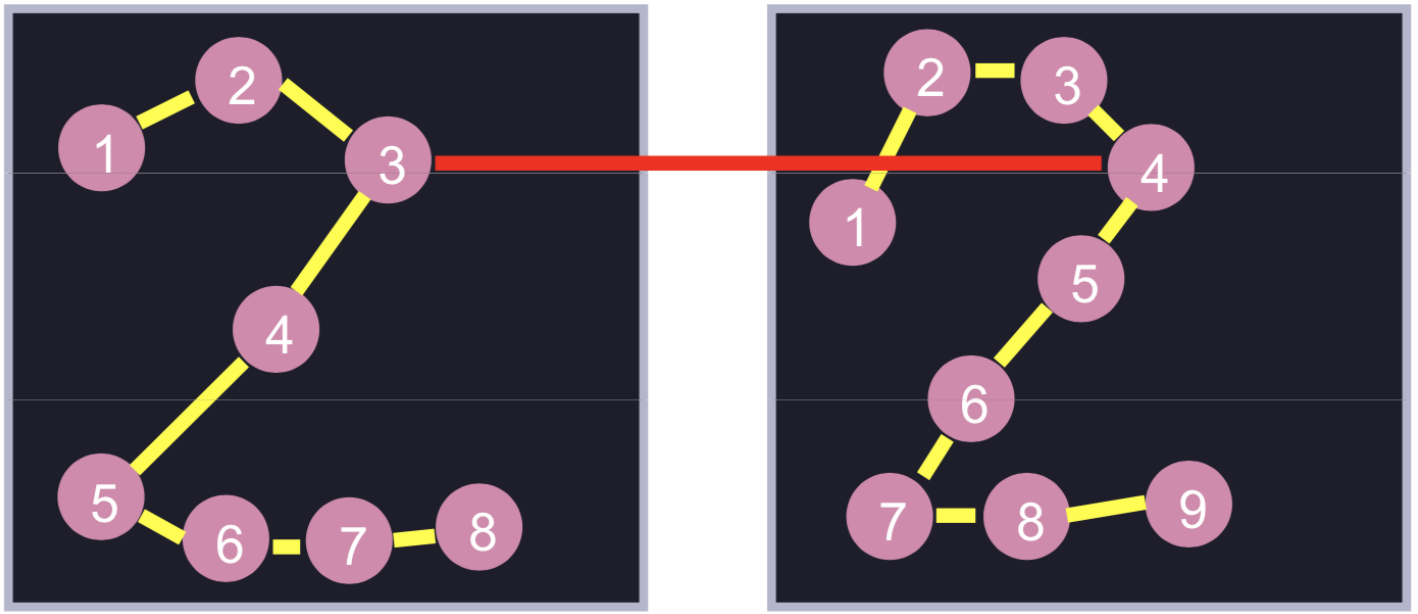


- What is the cost of alignment?

$$C = cost(s_1, t_2) + cost(s_2, t_2) + \cdots + cost(s_m, t_n)$$

- We could use the Euclidean distance: $cost(s_i, t_i) = d_{L_2}(s_i, t_i)$

Matching trajectories

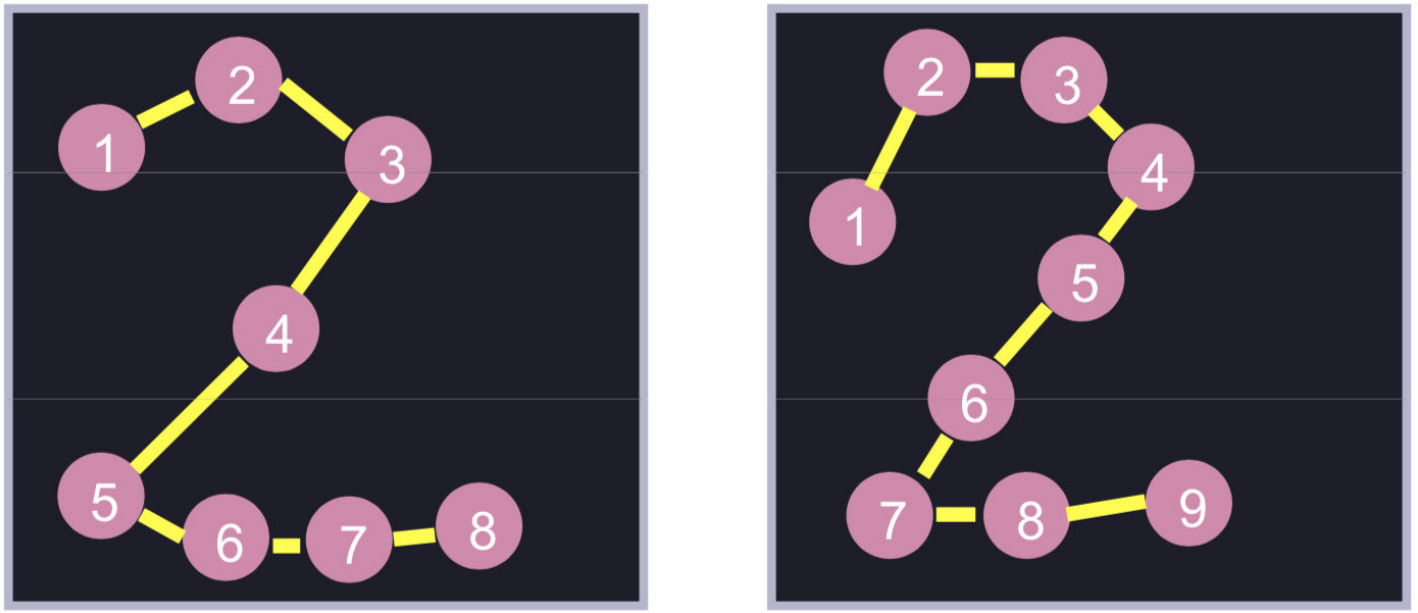


- What is the cost of alignment?

$$C = cost(s_1, t_1) + cost(s_2, t_2) + \cdots + cost(s_m, t_n)$$

- We could use the Euclidean distance: $cost(s_i, t_i) = d_{L_2}(s_i, t_i$
- Example: $cost(3,4) = d_{L_2}(M_3, Q_4)$

Matching trajectories

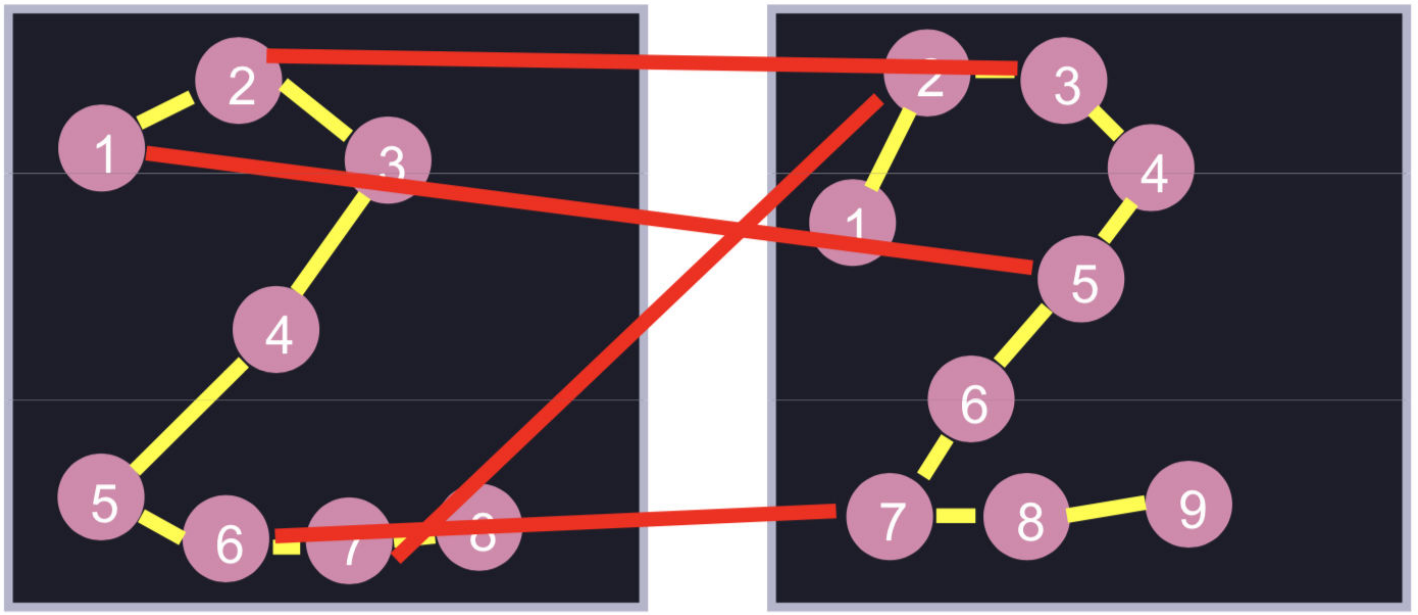


- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- What are the rules of alignment?

Matching trajectories



- We can align them:

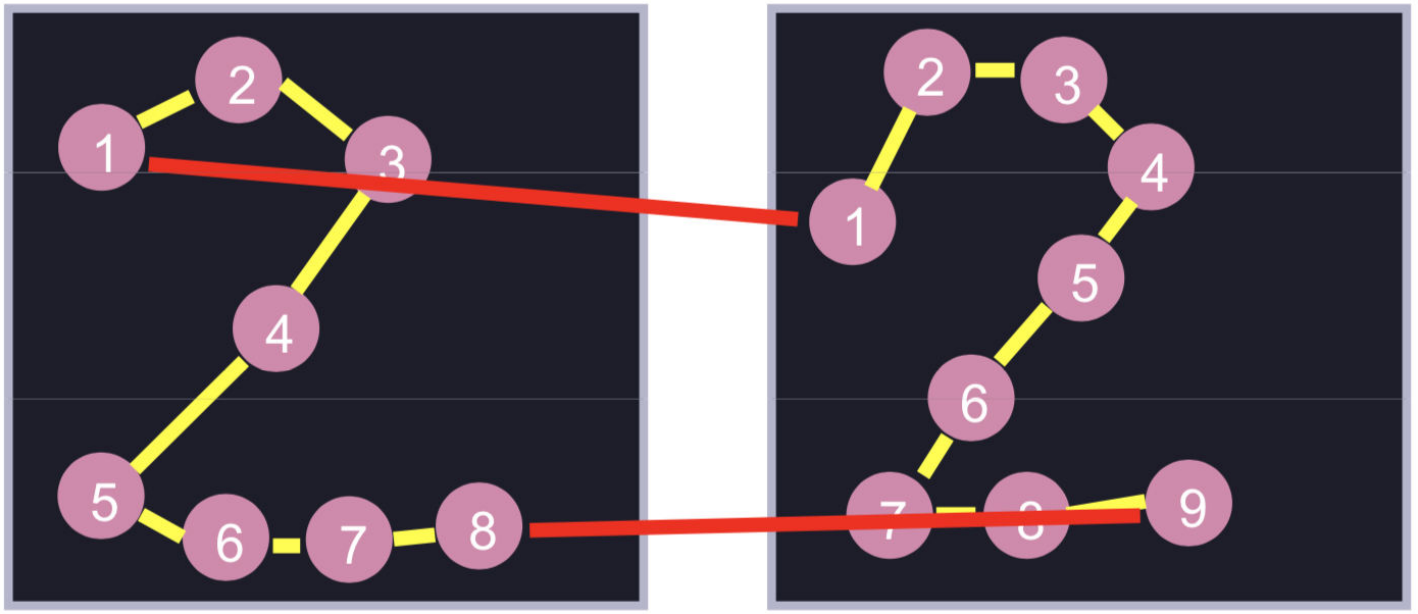
((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- What are the rules of alignment?

➢ Is alignment ((1, 5), (2, 3), (6, 7), (7, 1)) legal?

➢ Depends on what makes sense in our application

Rules of alignment for DTW

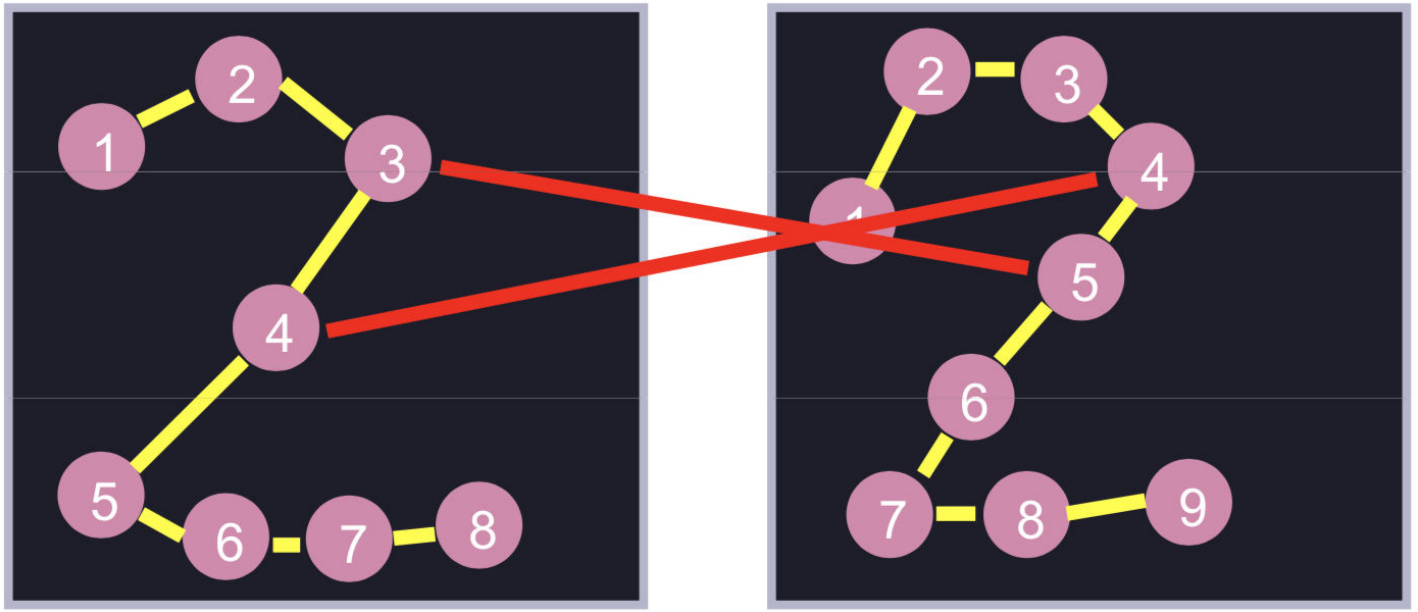


- We can align them:

((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- DTW rules: boundaries
  - First elements match: (s_1,t_1)
  - Last elements match: (s_m,t_n)

Rules of alignment for DTW



- Illegal alignment (violating monotonicity):

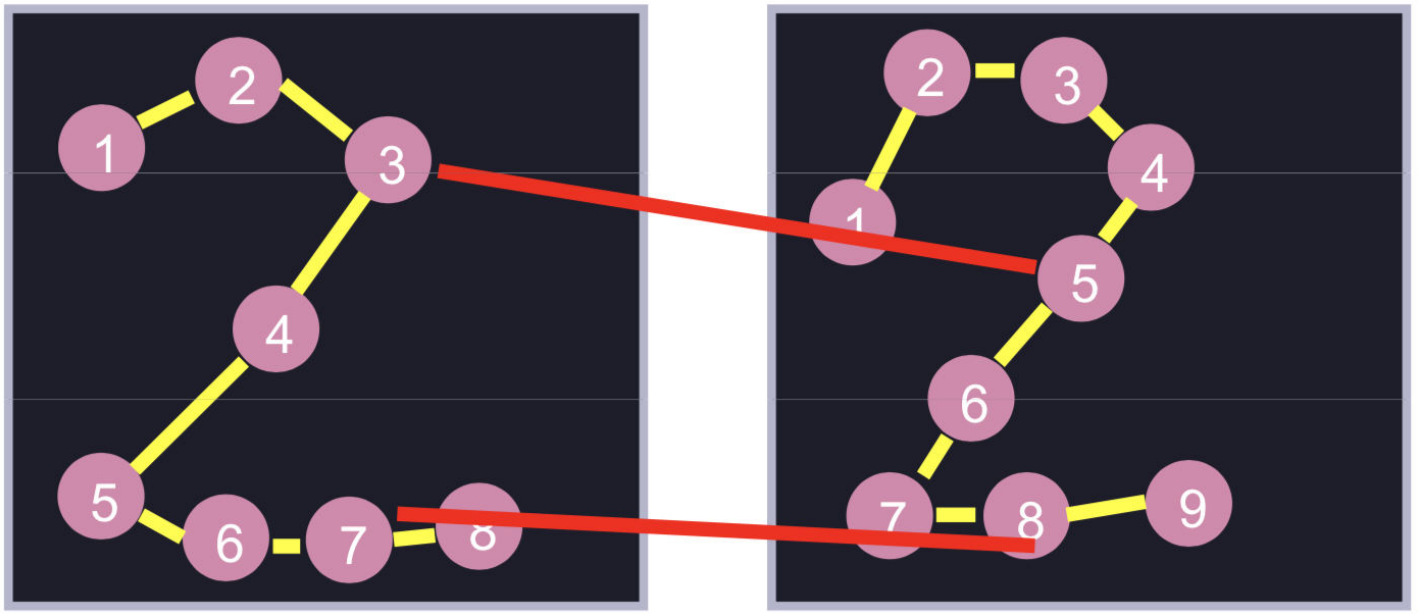
(..., (3, 5), (4, 4), ...)

- DTW rules: monotonicity (the alignment cannot go backwards)

➢ $0 \leq (s_{i+1} - s_i)$

➢ $0 \leq (t_{i+1} - t_i)$

Rules of alignment for DTW



- Illegal alignment (violating continuity):

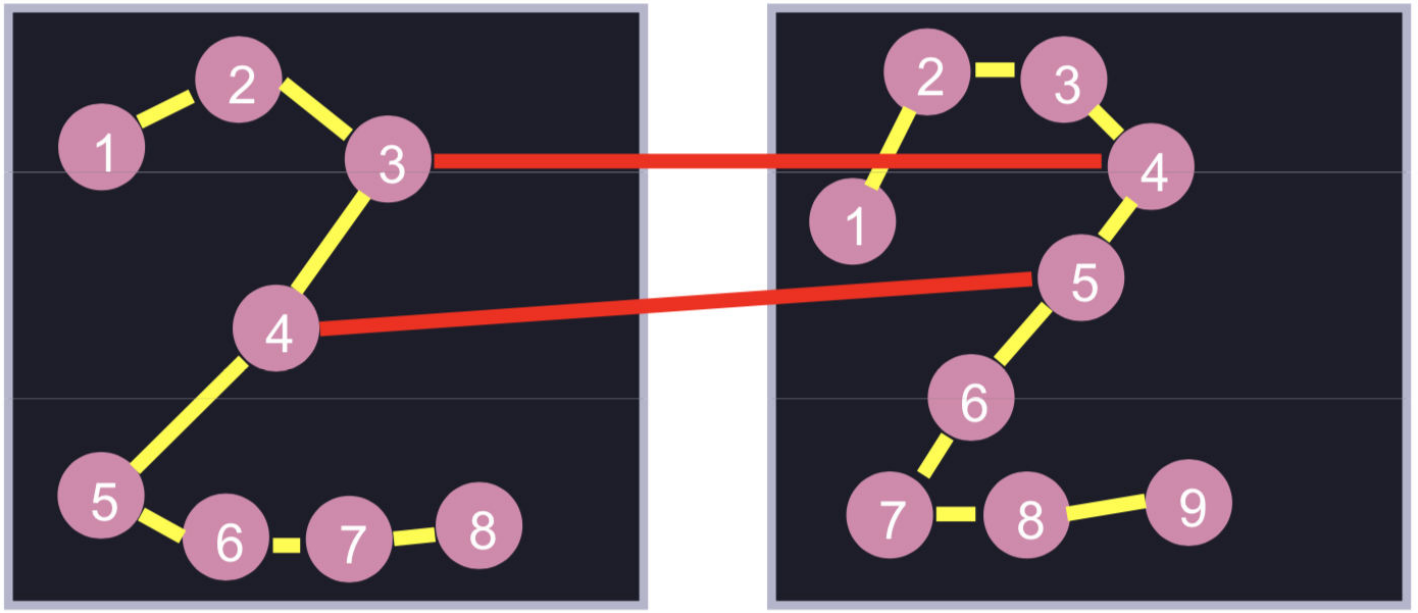
(..., (3, 5), (7, 8), ...)

- DTW rules: continuity (the alignment cannot skip elements)

➢ $(s_{i+1} - s_i) \leq 1$

➢ $(t_{i+1} - t_i) \leq 1$

Rules of alignment for DTW



- Valid alignment:

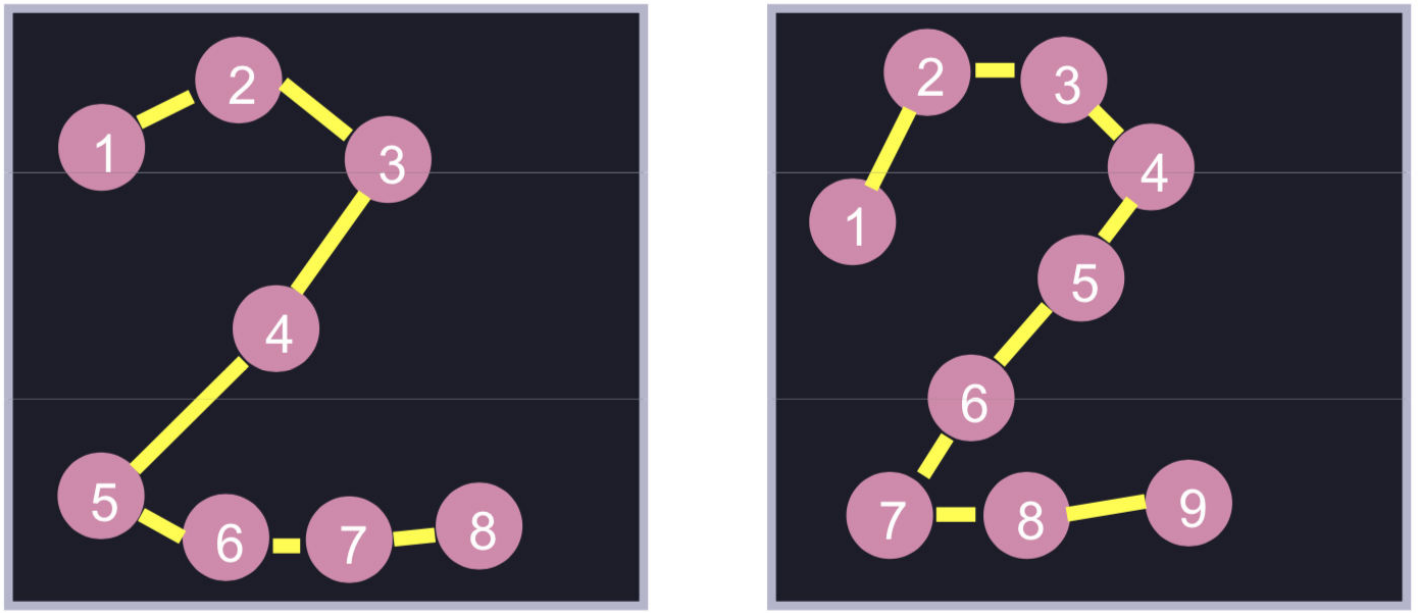
((1, 1), (2, 2), (2, 3), (3, 4), (4, 5), (4, 6), (5, 7), (6, 7), (7, 8), (8, 9))

- DTW rules: monotonicity and continuity

➢ $0 \leq (s_{i+1} - s_i) \leq 1$

➢ $0 \leq (t_{i+1} - t_i) \leq 1$

Dynamic Time Warping

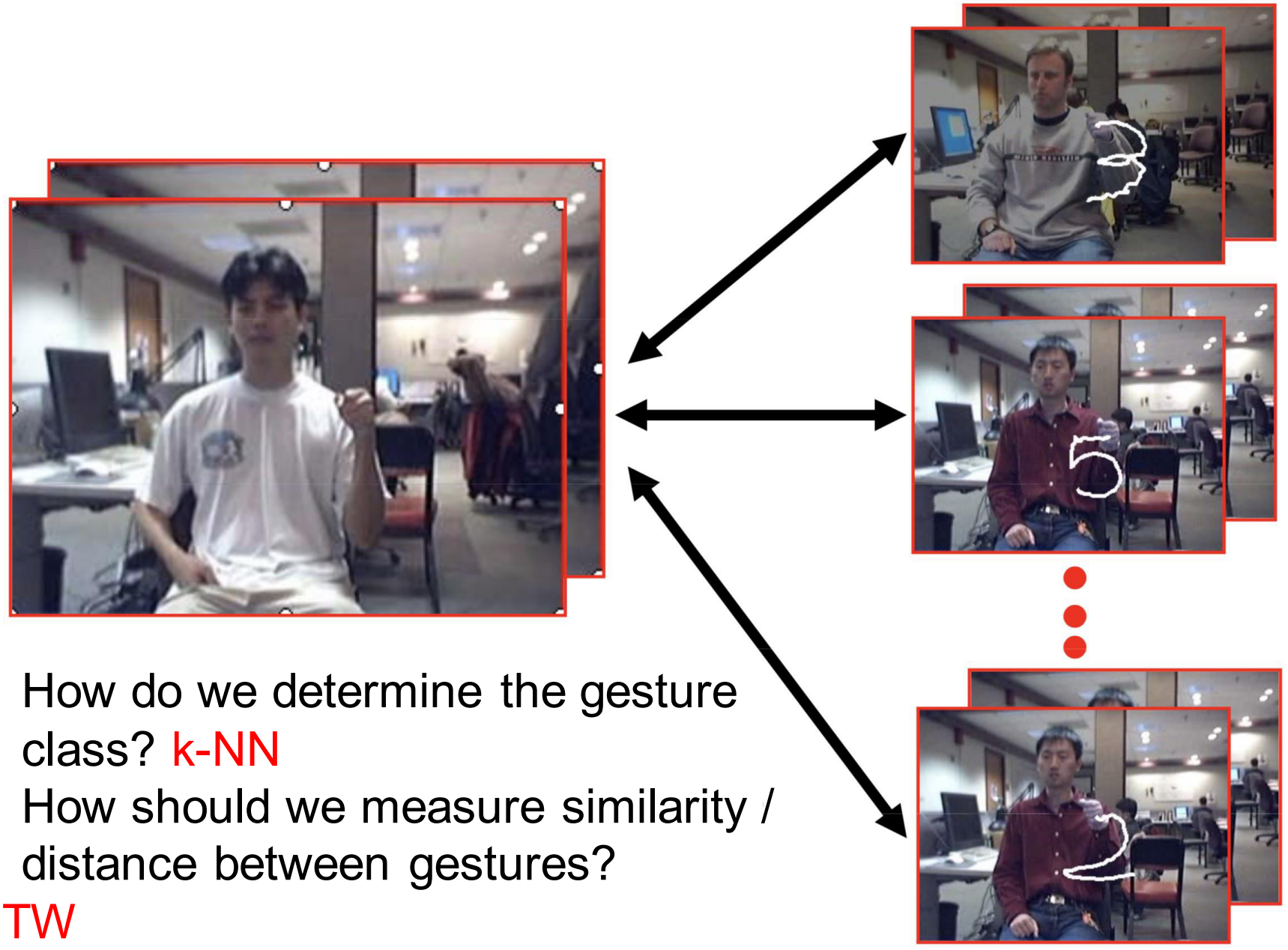


• Dynamic Time Warping (DTW) is a distance measure between sequences of points

• The DTW distance is the cost of the optimal alignment between two trajectories

➢ The alignment must obey the DTW rules defined in the previous slides

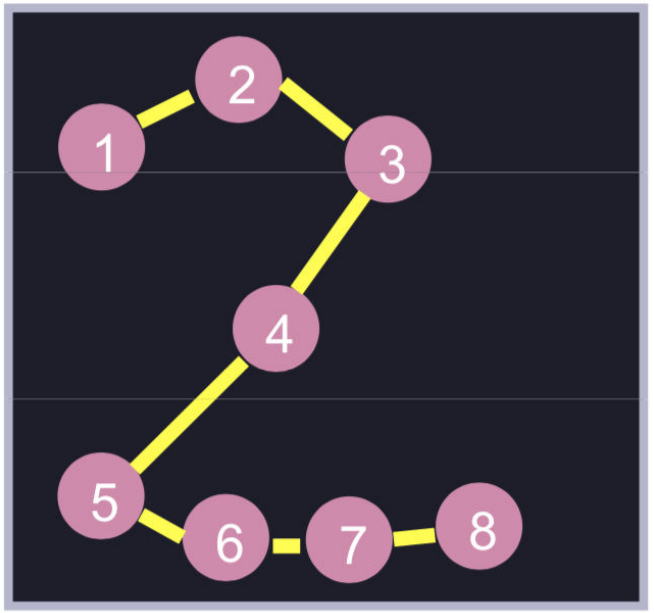
Gesture recognition



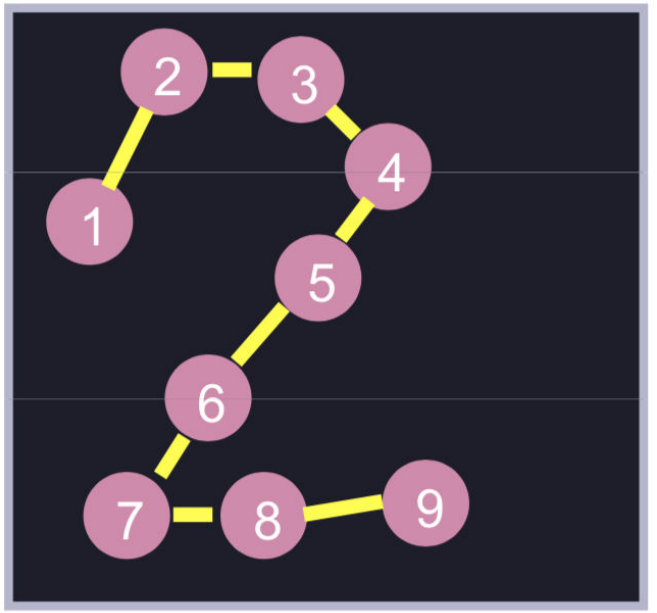
- How do we determine the gesture class? k-NN
- How should we measure similarity / distance between gestures?

DTW

Computing DTW (Edit) distance



M



Q

- Training sample: $M = (M_1, M_2, ..., M_8)$
- Test sample: $Q = (Q_1, Q_2, ..., Q_9)$
- Each M_i and Q_j can be, for example, a 2D pixel location of the hand (center of the bounding box)

Computing DTW (Edit) distance

- Training sample: $M = (M_1, M_2, ..., M_8)$
- Test sample: $Q = (Q_1, Q_2, ..., Q_9)$
- We want optimal alignment between M and Q
- Dynamic programming strategy:

➢ Break problem up into smaller, interrelated problems P(i,j), which we solve using a recursive relation

➢ Problem P(i,j): find optimal alignment between

$(M_1, M_2, ..., M_i)$ and $(Q_1, Q_2, ..., Q_j)$

Computing DTW (Edit) distance

- Solve problem P(1, j):
  - The optimal alignment is: ((1, 1), (1, 2), ..., (1, j))
- Solve problem P(i, 1):
  - The optimal alignment is: ((1, 1), (2, 1), ..., (i, 1))
- Solve problem P(i, j):
  - Find best solution from:

(i, j-1), (i-1, j), (i-1, j-1)

  - Add the pair (i, j) to the solution best solution from above

The DTW algorithm

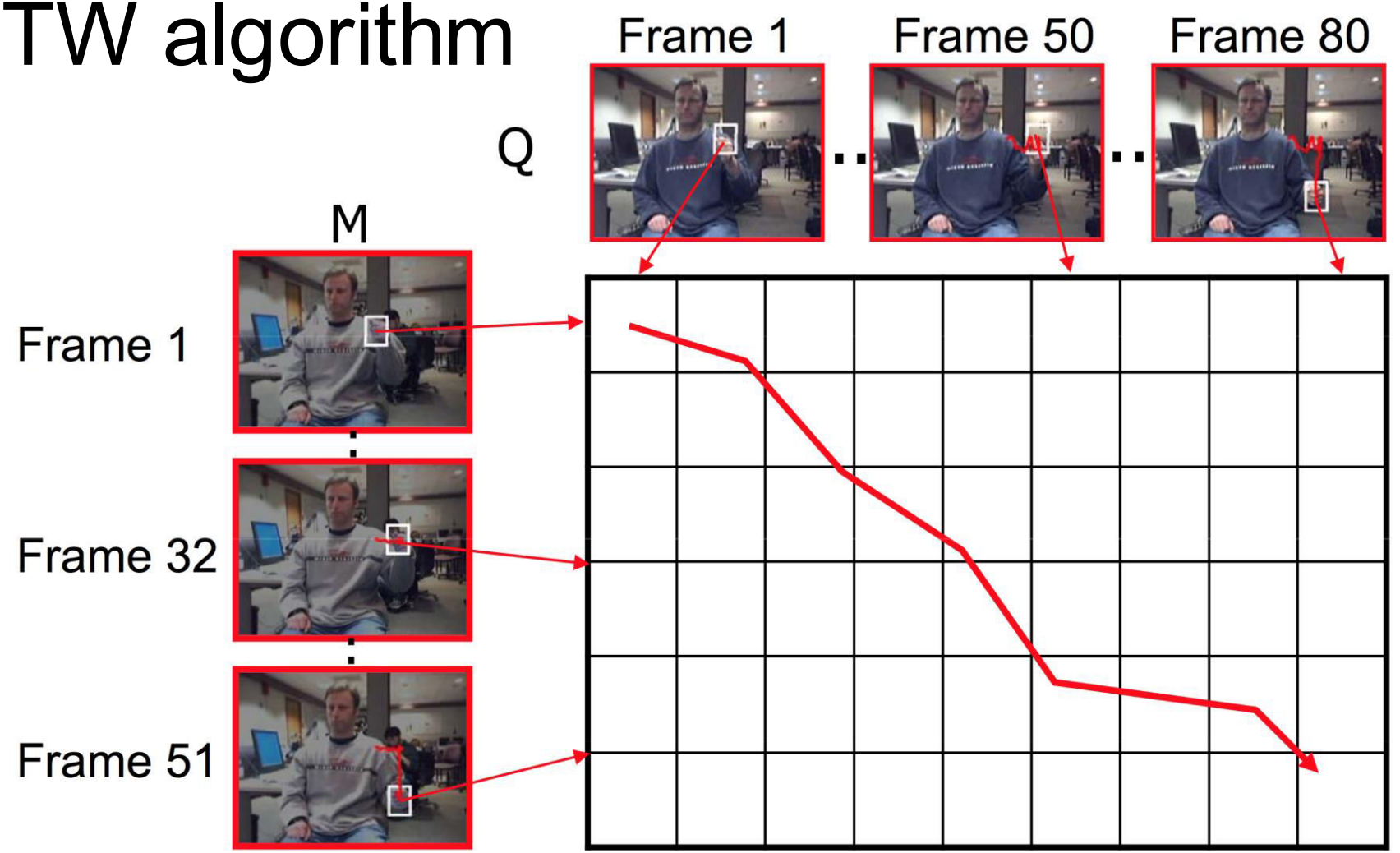
- Input:
  - Training sample: $M = [M_1, M_2, ..., M_8]$
  - Test sample: $Q = [Q_1, Q_2, ..., Q_9]$
- Algorithm:

```
C = np.zeros((m, n))
C[0,0] = cost(M1,Q1)
for i in range(1,m):
  C[i,0] = C[i-1,0] + cost(Mi,Q1)
for j in range(1,n):
  C[0,j] = C[0,j-1] + cost(M1,Qj)
for i in range(1,m):
  for j in range(1,n):
    C[i,j] = cost(Mi,Qj) + np.min(C[i-1,j],C[i,j-1],C[i-1,j-1])
```

- Return:

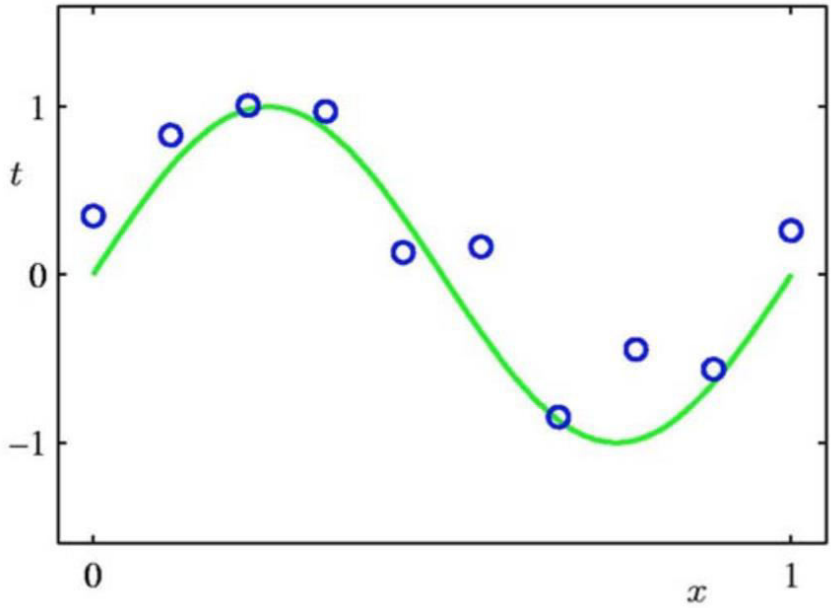
C[m,n]

The DTW algorithm



- For each cell (i, j):
  - Compute optimal alignment of M[1:i] and Q[1:j]
  - Answer depends only on (i-1, j), (i, j-1), (i-1, j-1)
  - Time: linear to size of table, quadratic to length of gestures

Regression from labeled samples



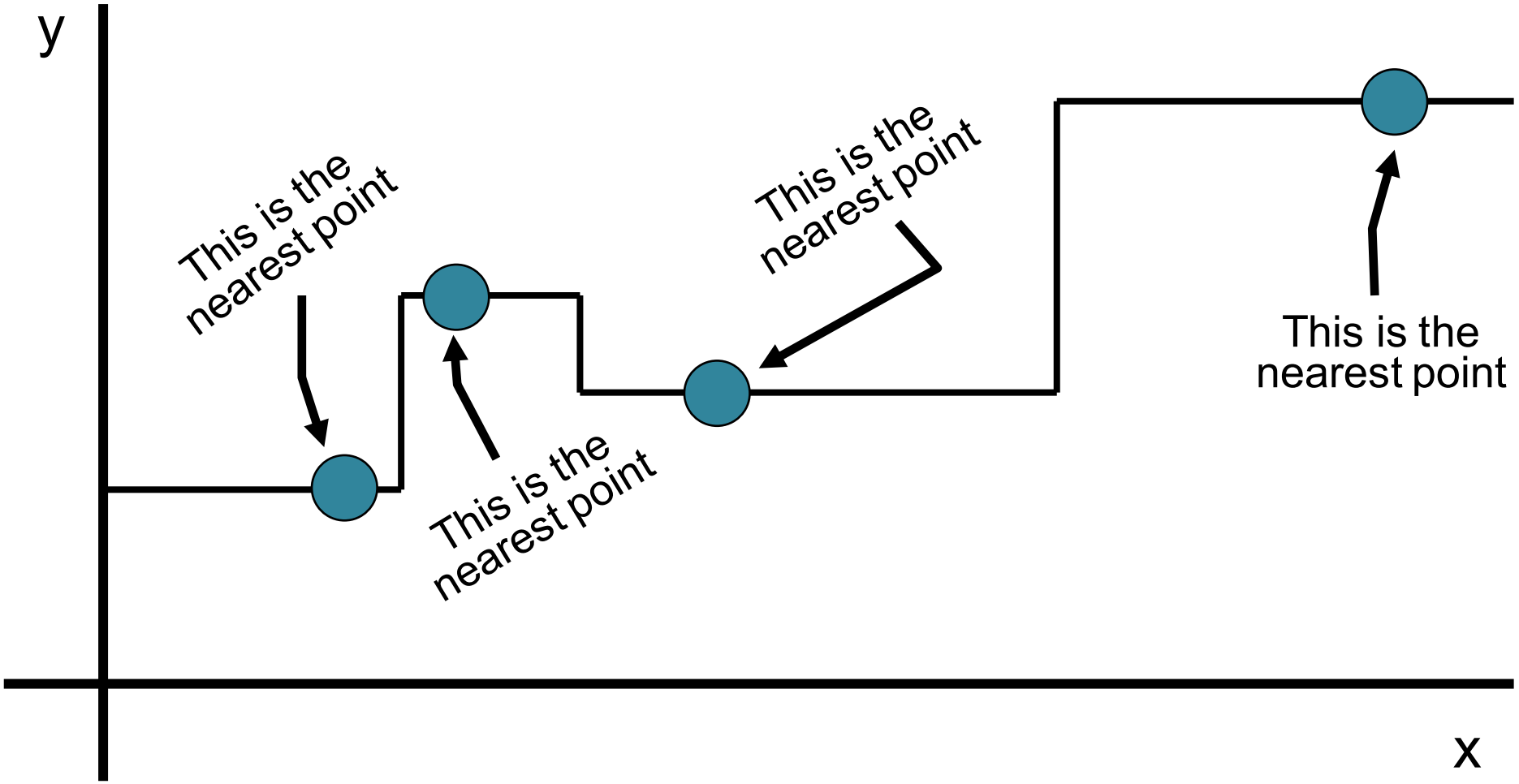
- Suppose we have a set of N training examples:

$(x_1, \ldots, x_N)$ and $(y_1, \ldots, y_N), x_i, y_i \in \mathbb{R}$

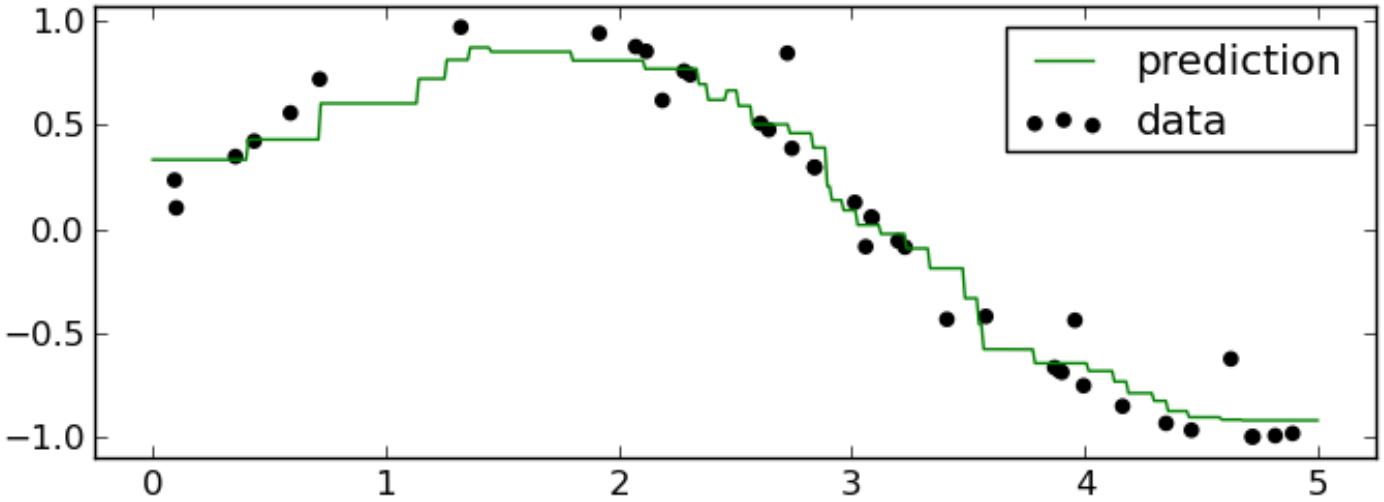
- The regression problem consists of estimating the function g(x) such that:

$$g(x_i) = y_i$$

1-NN for regression tasks



k-NN for regression tasks



- k-NN regression algorithm:

1) For each test sample x, we find the nearest k neighbors and their labels

2) The output-ul is the mean of the labels of the k neighbors:

$$f(\mathbf{x}) = \frac{1}{K} \sum_{i=1}^{K} y_i$$

Advantages and properties of k-NN

- k-NN is a very simple model
- Can be directly applied to multi-class problems
- The decision boundary is non-linear
- The quality of the results grows with the number of training samples
- We have a single parameter that requires tuning (k)
- The training error grows with k, but the decision boundary becomes smoother:

➢ Regularization method that increases the generalization capacity (to some extent)

Disadvantages of k-NN

- What does nearest mean? We have to define a distance
- Is the Euclidean distance always the best choice?
- The computational cost is quite high: we need to store and pass through the whole training set during inference (at test time)
- Possible solutions to avoid the high computational time:

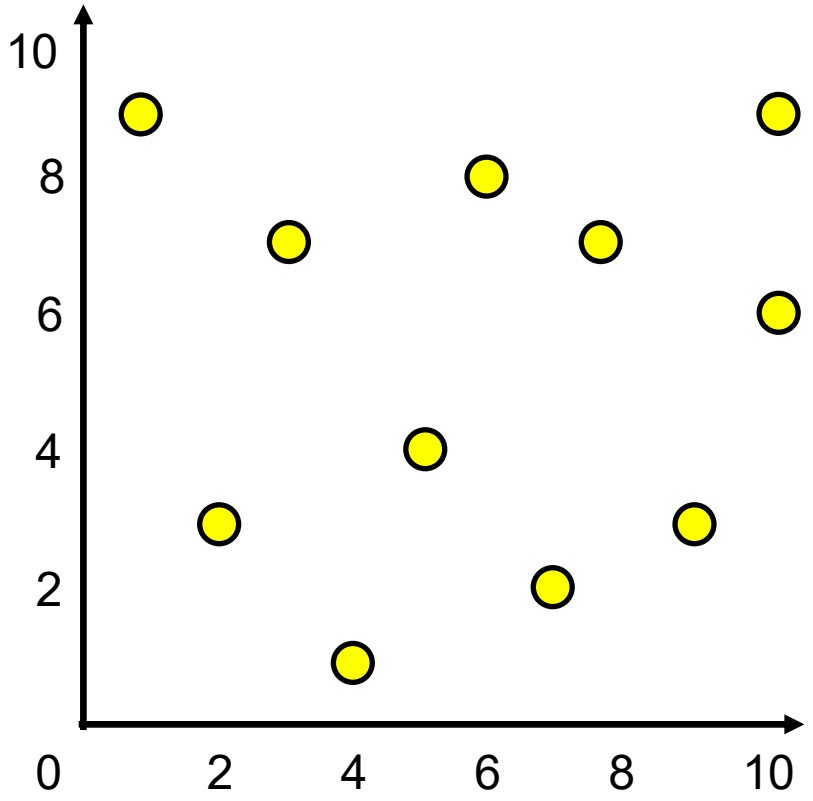
➢ Partition the feature space using k-d trees

➢ Use locality sensitive hashing

- Suffers from the “curse of dimensionality”

Approximate k-NN based on k-d tree

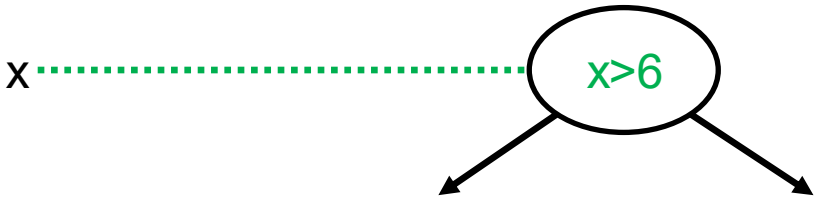
- Build a k-d tree from training data:

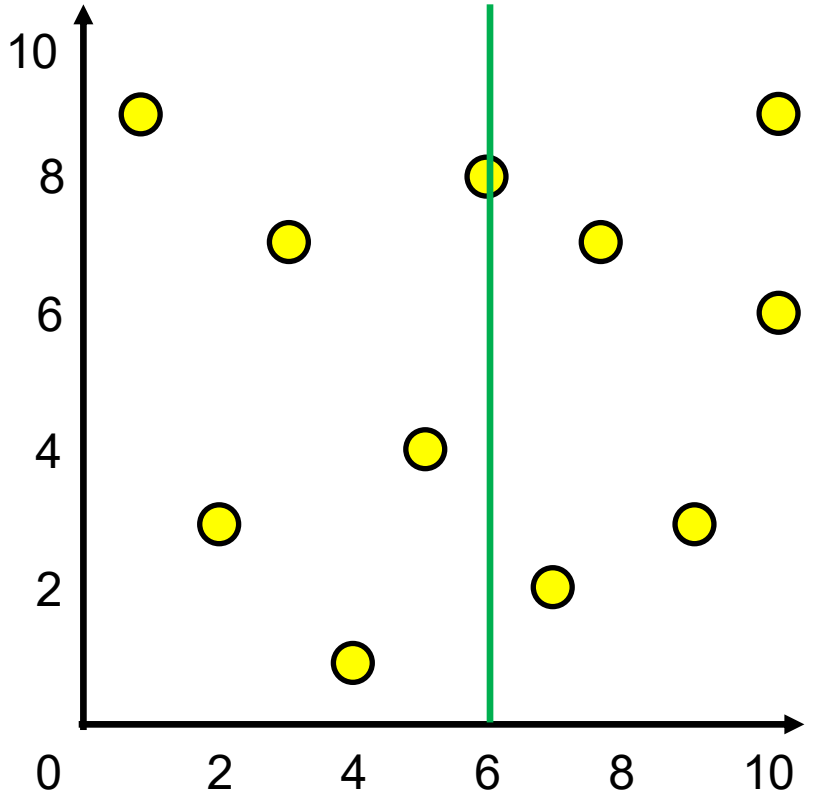


Approximate k-NN based on k-d tree

- Build a k-d tree from training data:

pick random/alternate dimension, find median, split data, repeat





Approximate k-NN based on k-d tree

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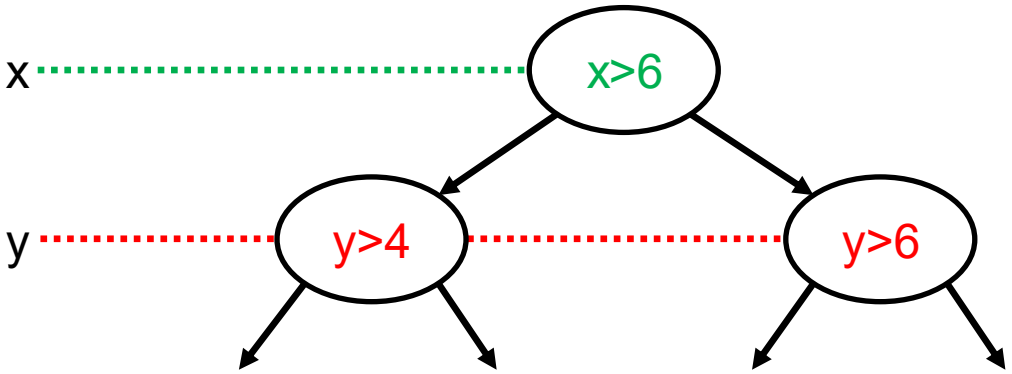
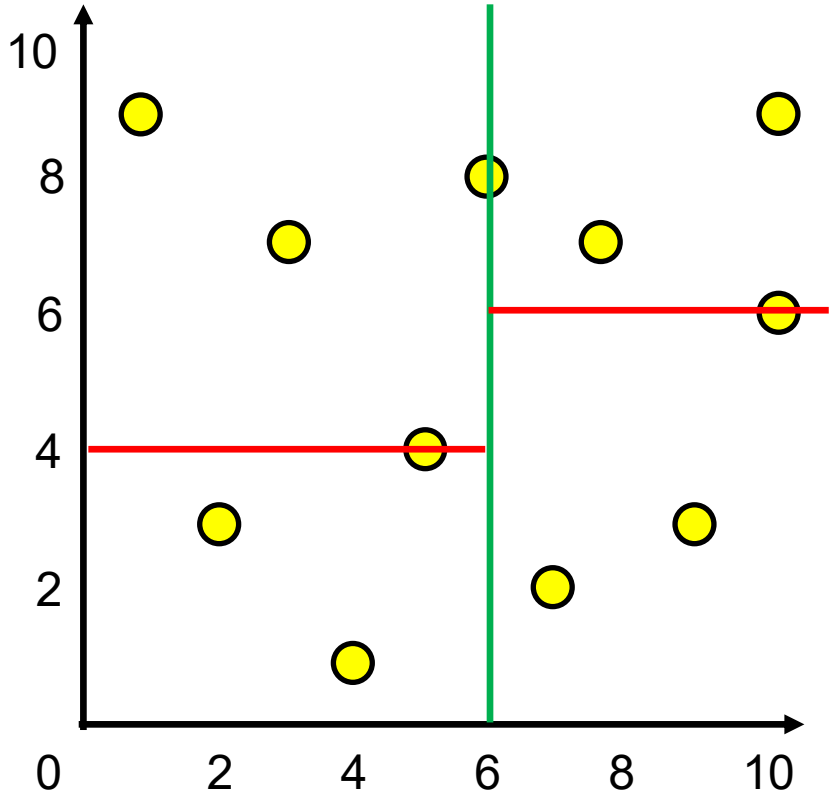
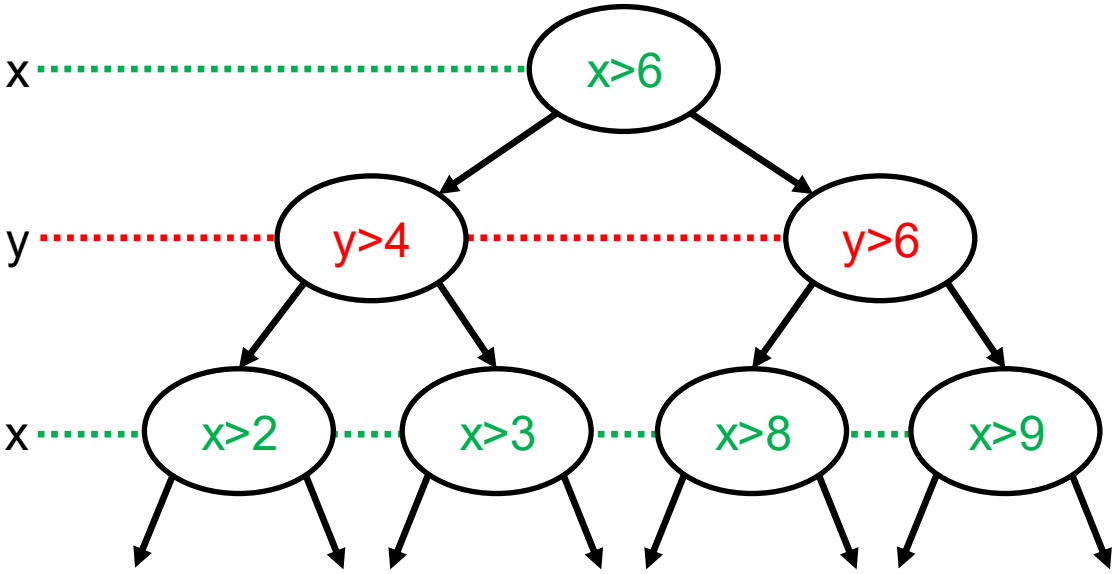


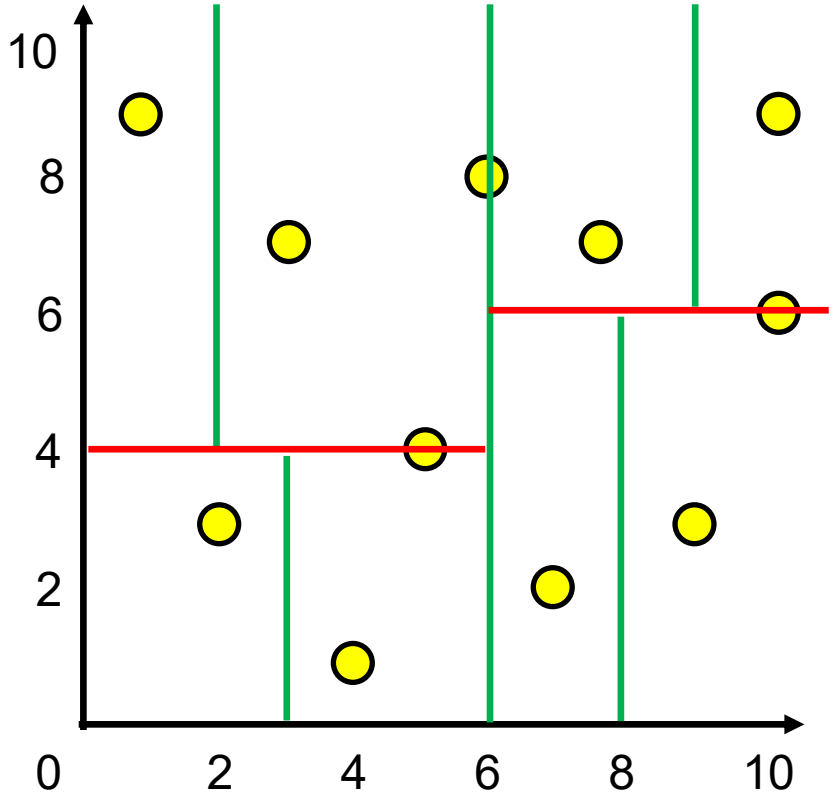


Approximate k-NN based on k-d tree

- Build a k-d tree from training data:

pick random/alternate dimension, find median, split data, repeat





Approximate k-NN based on k-d tree

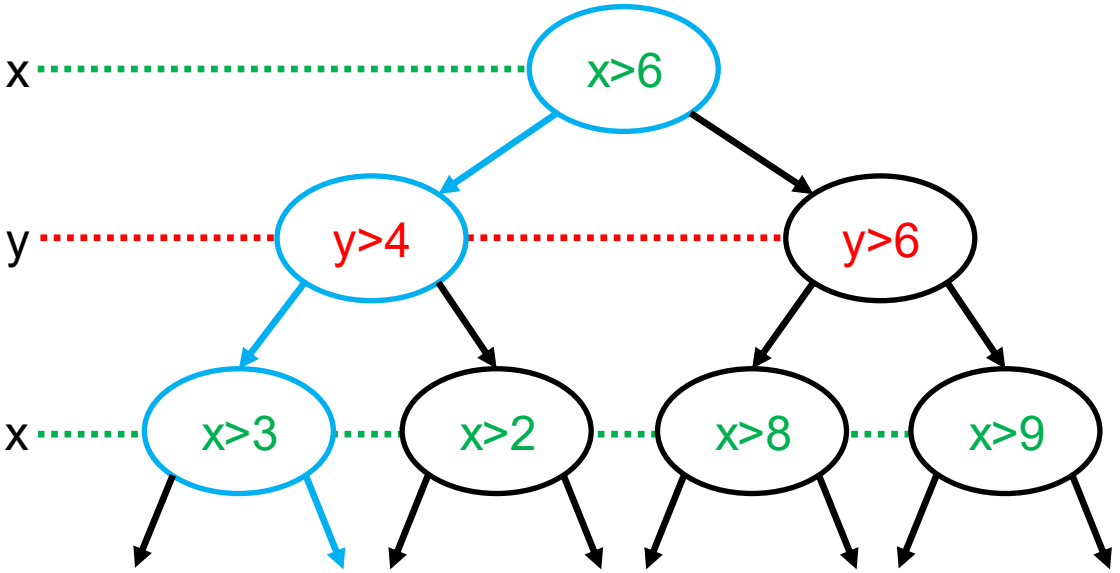
- Build a k-d tree from training data:

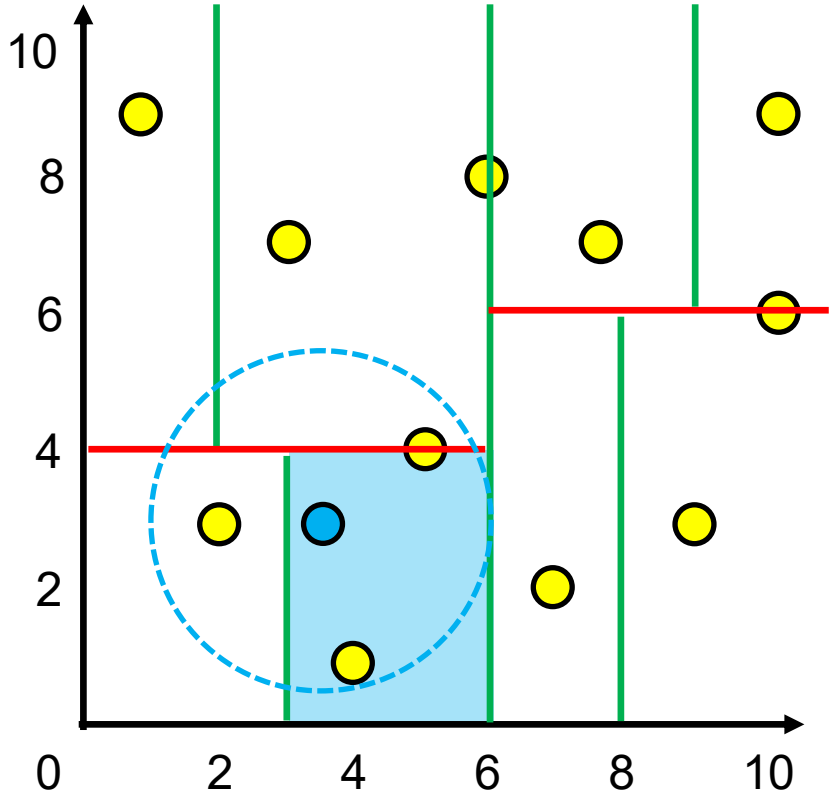
pick random/alternate dimension, find median, split data, repeat

- Find NN for test sample:

1) Find region containing test point

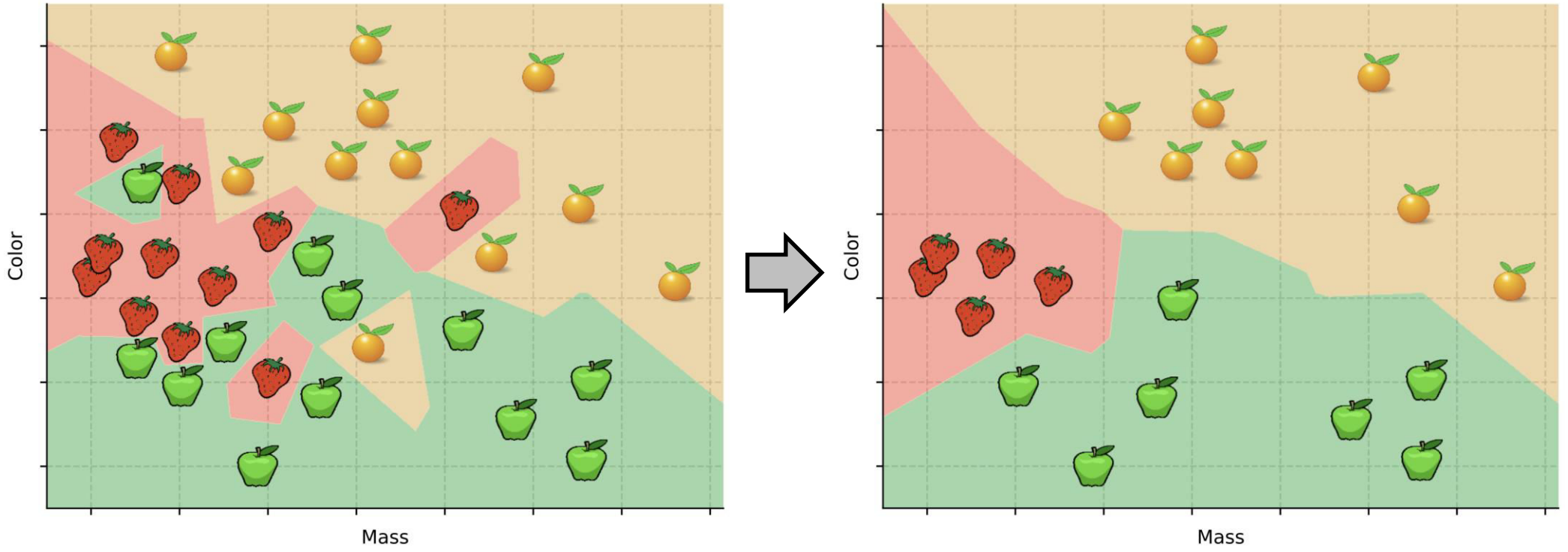
2) Compare to all points in region





Edited Nearest Neighbors

- Eliminate training samples that have a different label from its nearest k neighbors
- Regularization technique that produces smooth border by removing training outliers

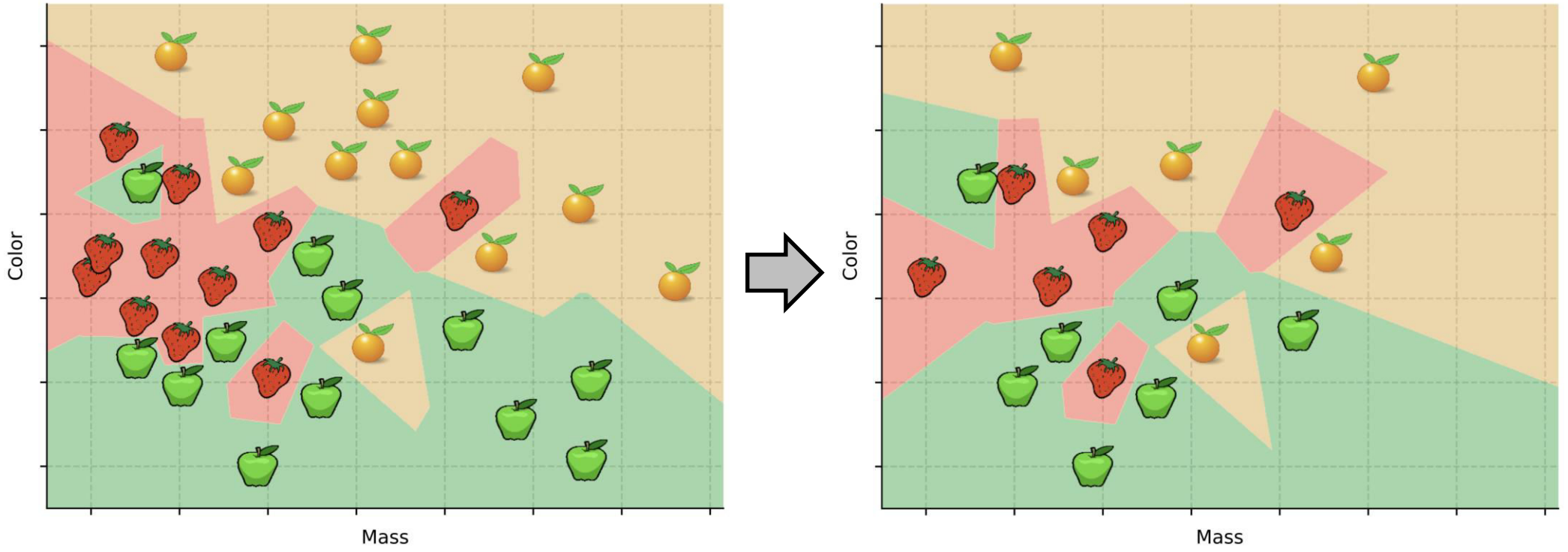


Condensed Nearest Neighbors

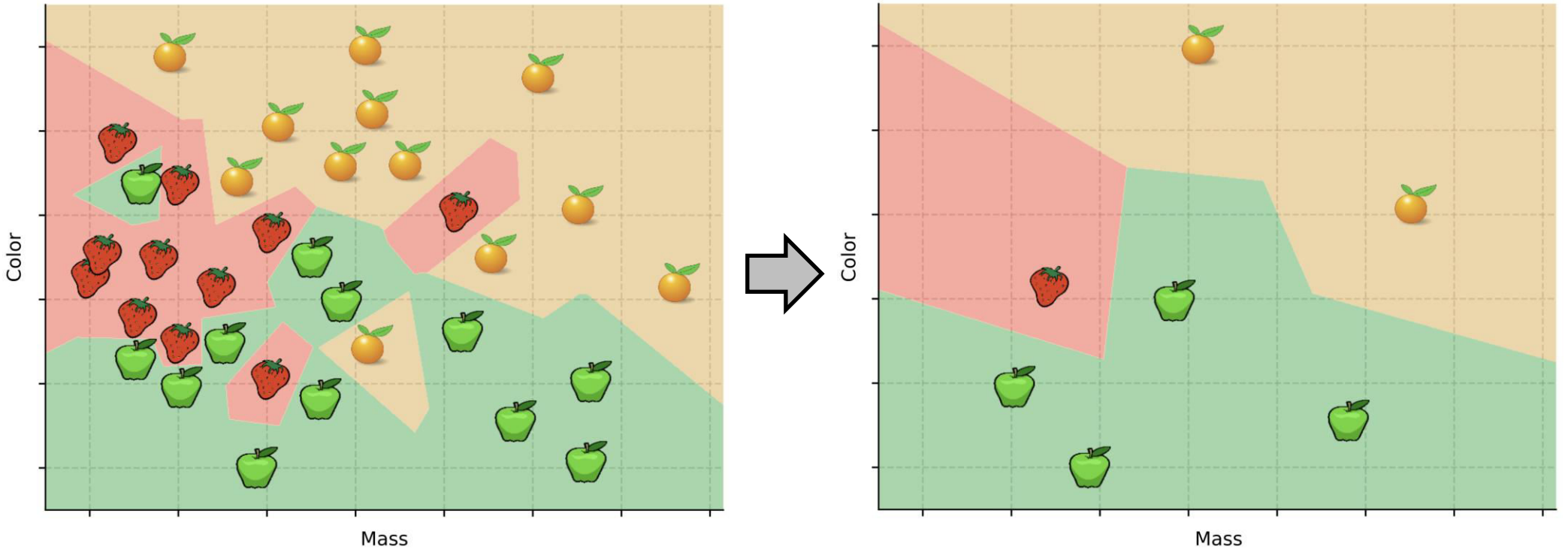
- Eliminate training samples that have no effect on the decision boundary
- Algorithm:

1) Randomly select a set P of samples, at least one for each class

2) Each training sample that is not in P should be added to P, if the k-NN based on P classifies it incorrectly



Edited + Condensed Nearest Neighbors



Local Learning

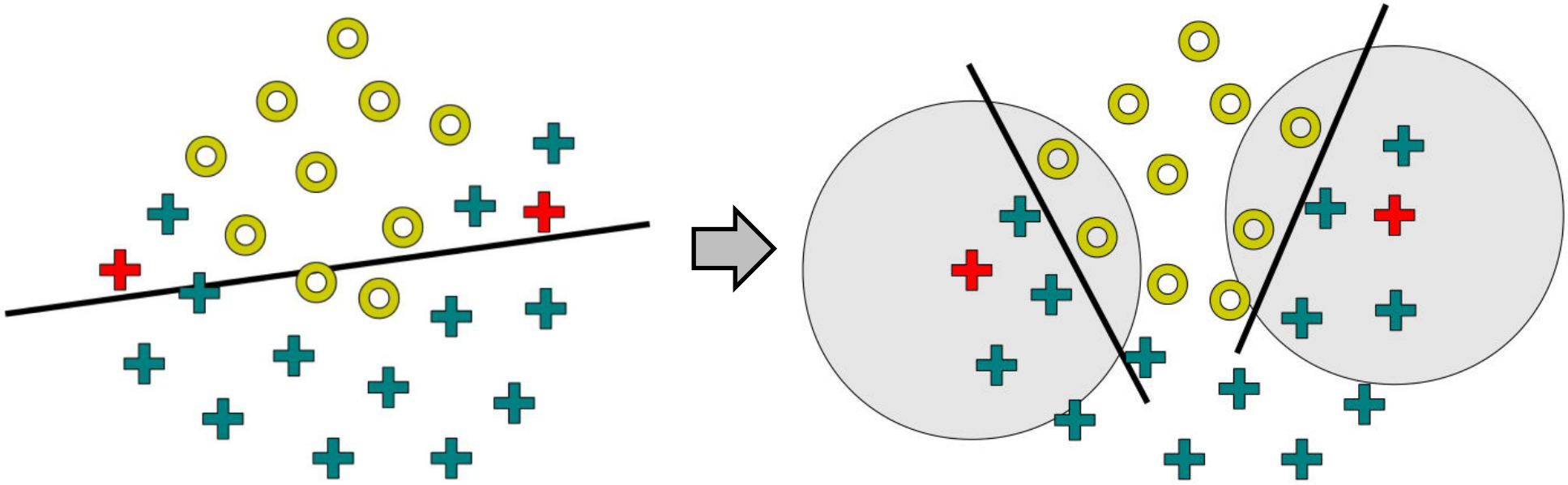
Local Learning

- Local learning algorithm:

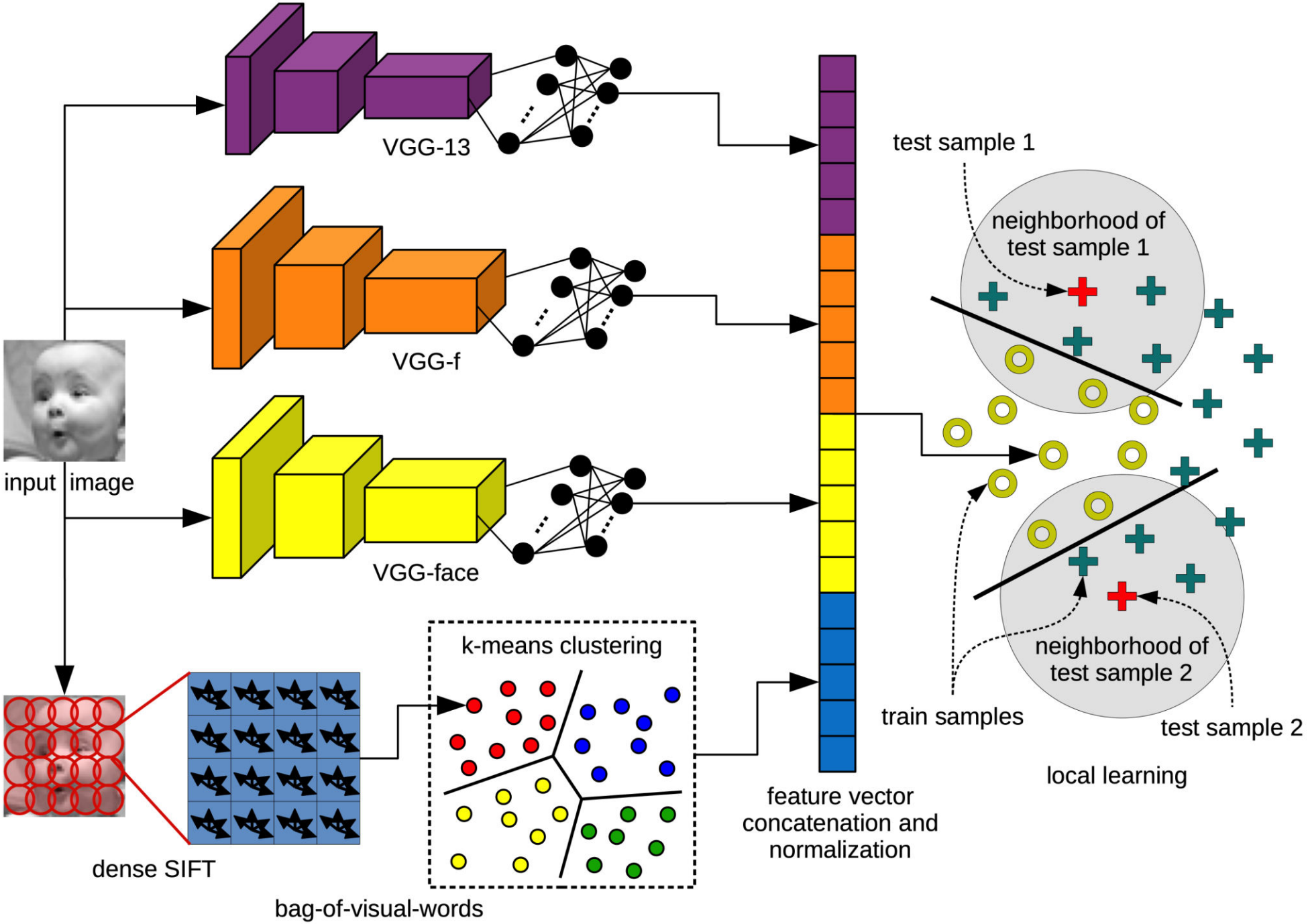
1) select training samples located in the vicinity of the given test sample

2) train a classifier on the selected examples

3) apply the classifier to predict the class label of the test sample



Local Learning



Curse of Dimensionality

Curse of dimensionality

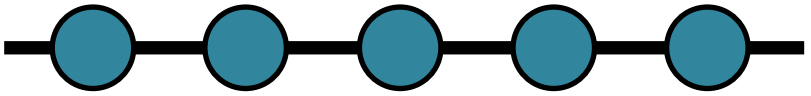
- In machine learning, we often use high-dimensional feature vectors
- Example:

➢ When we analyze gray-scale images of 200x200 pixels, then we are working with a feature space of 40.000 dimensions

➢ If the images are color (represented in the RGB or HSV color spaces), the dimensionality of the feature space grows to 120.000

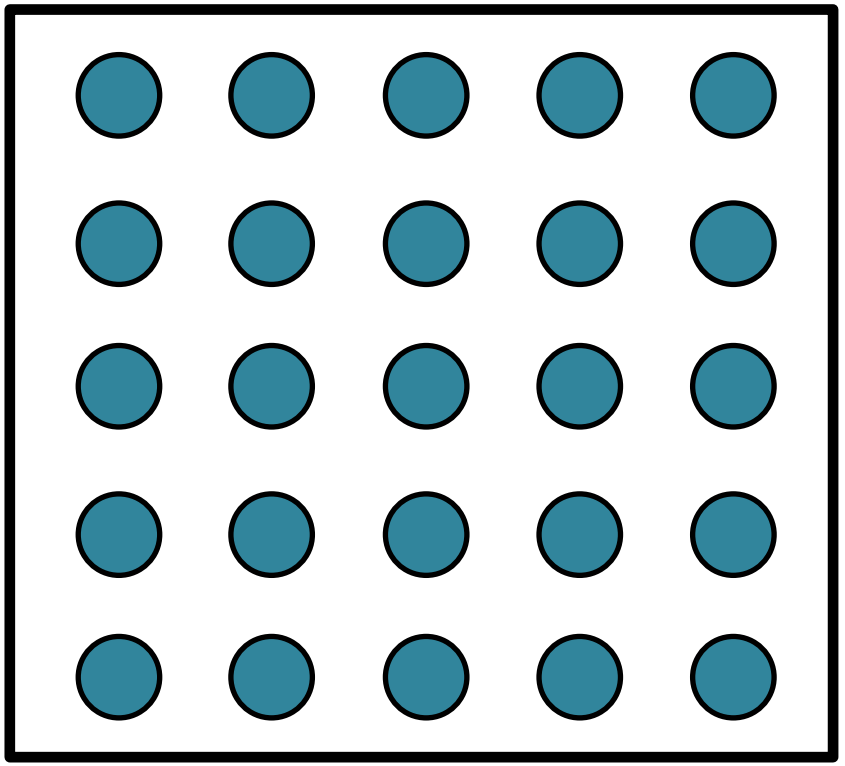
Curse of dimensionality

- To “fill” a 1D space (e.g. $\mathbb{R}^1$) we need 5 data points:



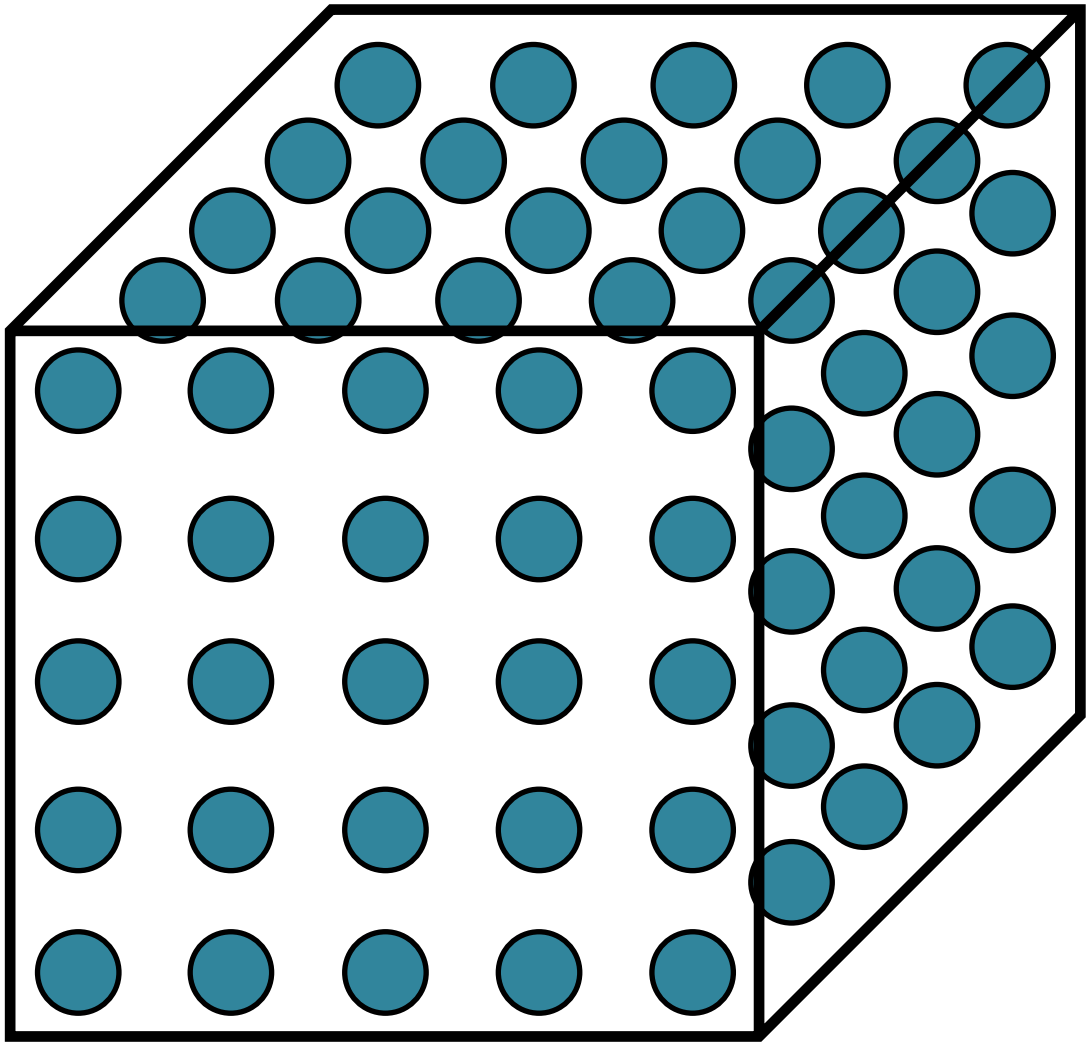
Curse of dimensionality

- To “fill” a 2D space (e.g. $\mathbb{R}^2$) we need 25 data points:



Curse of dimensionality

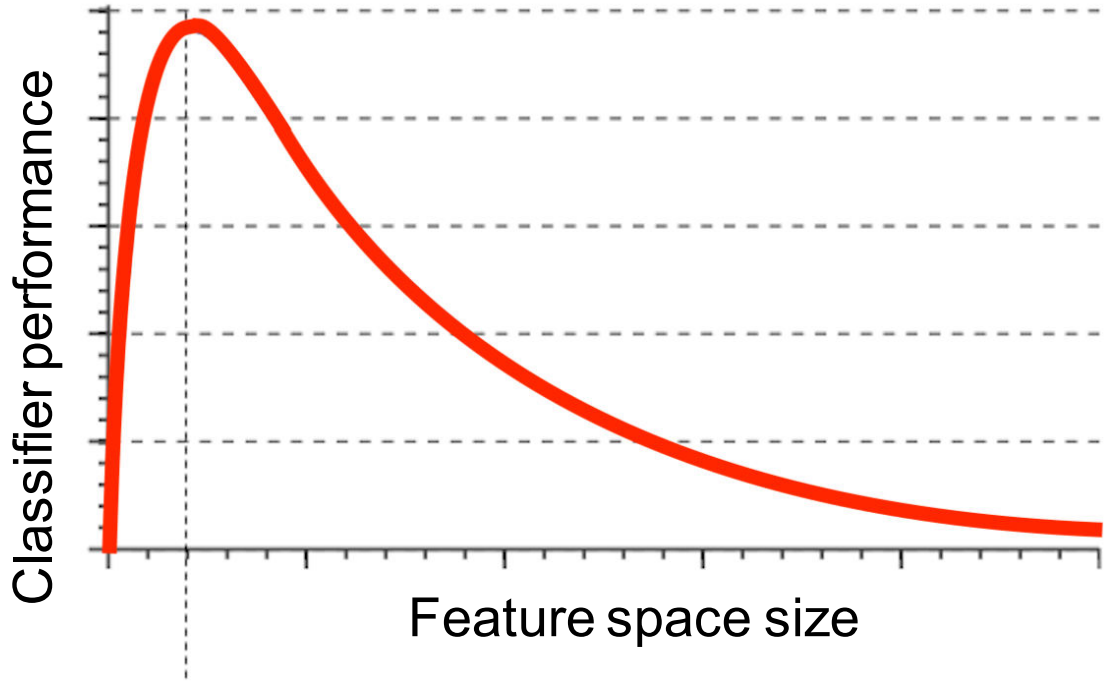
- To “fill” a 3D space (e.g. $\mathbb{R}^3$) we need 125 data points:



Curse of dimensionality

- To "fill" an nD space (e.g. $\mathbb{R}^n$) we need an exponential number of data points
- If we have a large number of features that describe our data, then the system requires an extremely large training set in order to learn a model with good generalization
- Most of the times, large training sets are not available in practice

Hughes phenomenon



- The Hughes phenomenon shows that, as the number of features grows, the performance of the classifier increases until we reach the optimal number of features
- Adding more features while keeping the size of the training set unchanged degrades the classifier performance

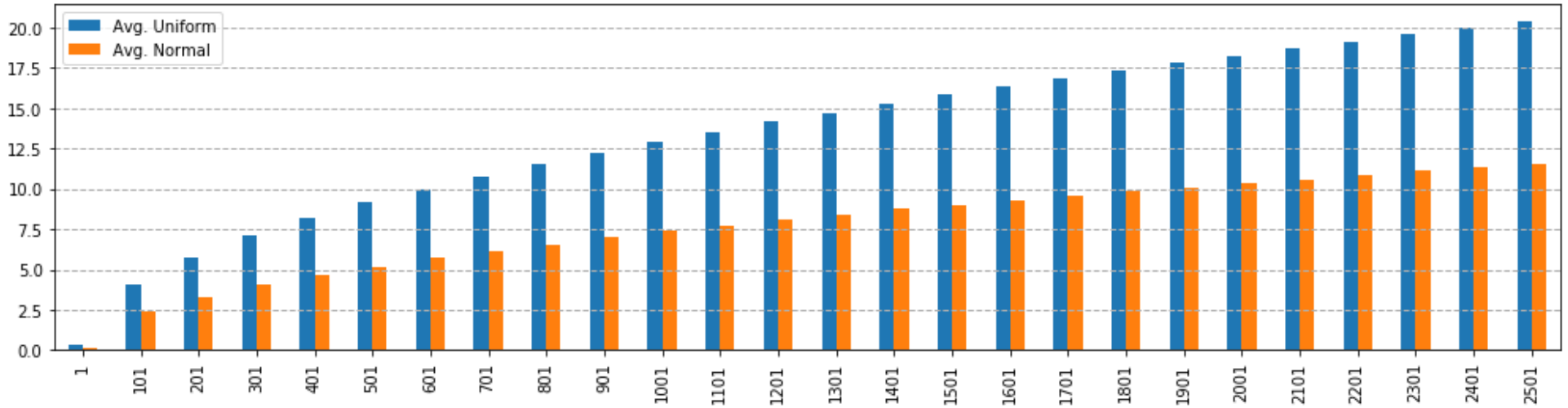
Curse of dimensionality

- Increasing the dimension of an Euclidean feature space, implies the addition of positive terms in the computation of the Euclidean distance:

$$(x, y) = \sqrt{(x_1 - y_1)^2 + \cdots + (x_n - y_n)^2}$$

- In other words, because the number of features grows for a fixed number of data samples, the feature space becomes increasingly sparse (less dense)

Curse of dimensionality



Average distance for 1000 points in the unit cube

- By increasing the feature space size, the average distance grows rapidly
- Hence, the more dimensions we have, the more data is necessary to overcome the curse of dimensionality!
- When the distance between observations increases, the learning task becomes more difficult, since the probability of finding training samples that are truly similar with the test sample decreases