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(Attendance Code: 406355)

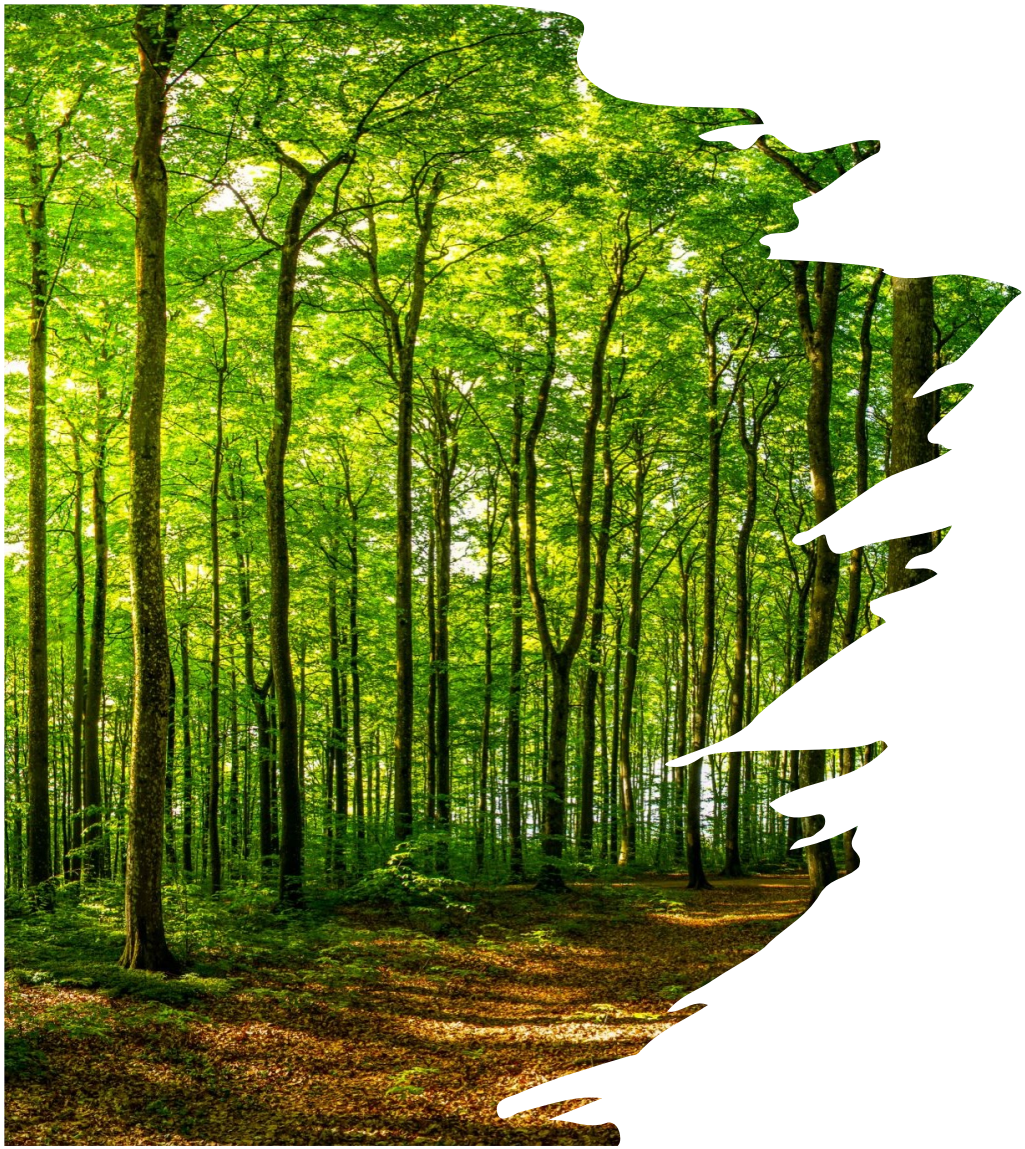
Lecture 10 -- K-Nearest Neighbour

Up to now,

Machine Learning Basic Knowledge

Safety and Reliability Properties (but the algorithms on how to attack and defend will be introduced later)

Decision Tree Learning



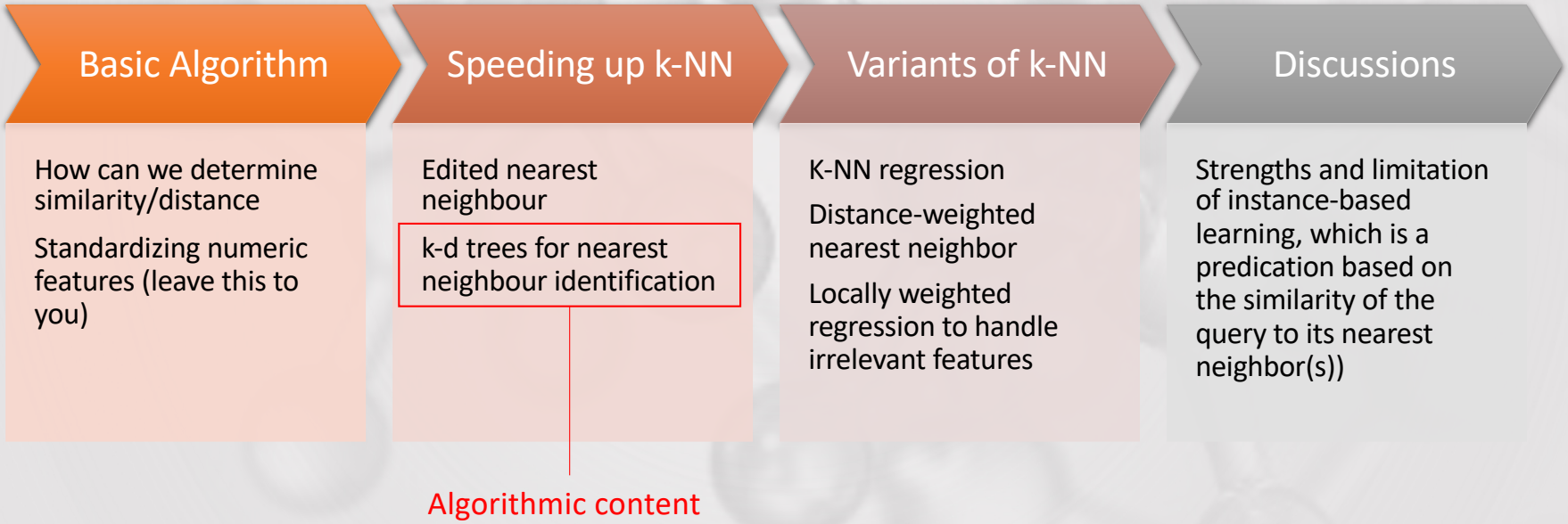
Confidence for decision tree (example)

- Random forest:
  - Multiple decision trees are trained, by using different resamples of your data.
  - Probabilities can be calculated by the proportion of decision trees which vote for each class.

- For example, if 8 out of 10 decision trees vote to classify an instance as positive, we say that the confidence is 8/10.

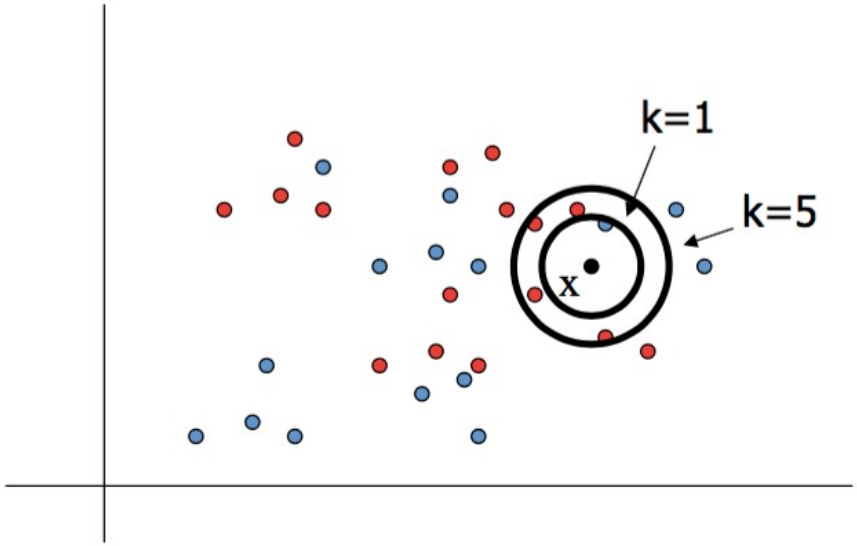
Here, the confidences of all classes add up to 1

Today's Topics – K-nearest neighbor



K-NN algorithm, illustrated

To classify a new input vector x, examine the k-closest training data points to x and assign the object to the most frequently occurring class



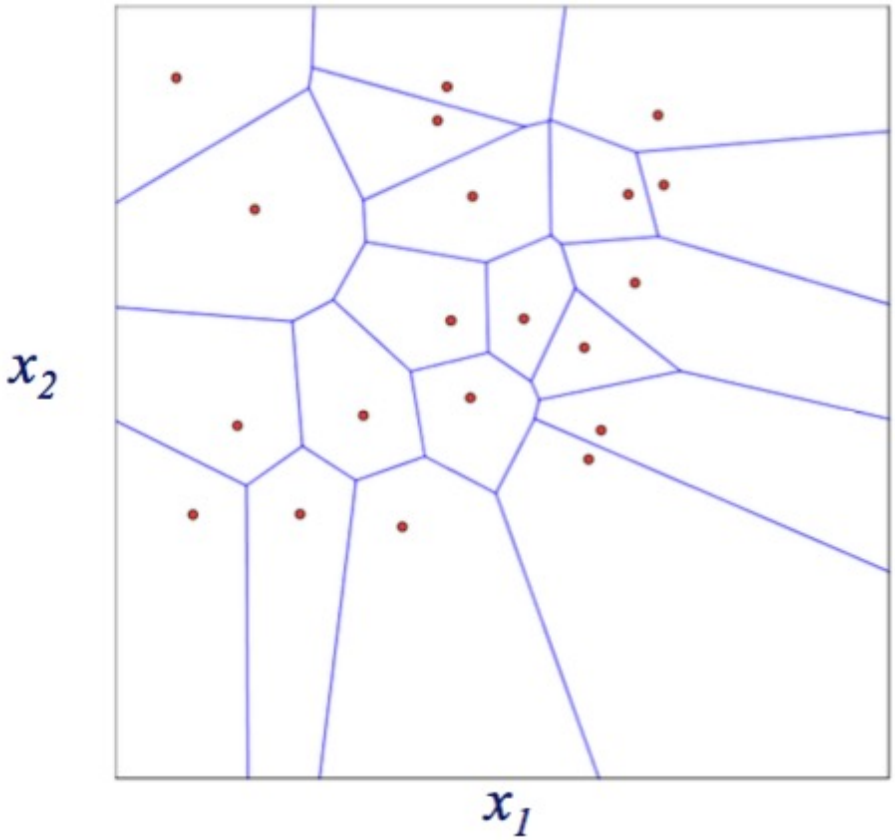
Nearest-neighbor classification

- Learning stage
  - Given a training set $(\mathbf{x}^{(1)}, y^{(1)}) \ldots (\mathbf{x}^{(m)}, y^{(m)})$, do nothing
    - (it's sometimes called a *lazy learner*)

- Classification stage
  - **given**: an instance $x^{(q)}$ to classify
  - find the training-set instance $x^{(i)}$ that is most similar to $x^{(q)}$
  - return the class value $y^{(i)}$

The decision regions for nearest-neighbor classification

- Voronoi diagram: each polyhedron indicates the region of feature space that is in the nearest neighborhood of each training instance



For the case when k=1 and we have two features X_1 and X_2

Nearest Neighbor

When to Consider

- Less than 20 attributes per instance
- Lots of training data

Advantages

- Training is very fast
- Learn complex target functions
- Do not lose information

Disadvantages

- Slow at query time
- Easily fooled by irrelevant attributes

k-nearest-neighbor classification: Algorithm

- classification task
  - **given**: an instance $x^{(q)}$ to classify
  - find the k training-set instances $(\mathbf{x}^{(1)}, y^{(1)}) \ldots (x^{(k)}, y^{(k)})$ that are the most similar to $x^{(q)}$
  - return the class value

$$\hat{y} \leftarrow \underset{v \in \text{values}(Y)}{\text{argmax}} \sum_{i=1}^{k} \delta(v, y^{(i)}) \qquad \delta(a,b) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise} \end{cases}$$

  - (i.e. return the class that has the most number of instances in the k training instances)

Example

- Suppose all features are categorical
  - Hamming distance (or L^0 norm): count the number of features for which two instances differ

- Example: X = (Weekday, Happy?, Weather) Y = AttendLecture?
  - D : in the table
  - New instance: <Friday, No, Rain>
  - Distances = {2, 3, 1, 2}
  - For 1-nn, which instances should be selected?
  - For 2-nn, which instances should be selected?
  - For 3-nn, which instances should be selected?

v1	**v2**	**v3**	**y**
Wed	Yes	Rain	No
Wed	Yes	Sunny	Yes
Thu	No	Rain	Yes
Fri	Yes	Sunny	No

New datum

Fri	No	Rain	

Example

- Example: X = (Weekday, Happy?, Weather) Y = AttendLecture?
  - New instance: <Friday, No, Rain>
  - For 3-nn, selected instances: {(<Wed, Yes, Rain>, No), (<Thu, No, Rain>, Yes), (<Fri, Yes, Sunny>, No)}
- Classification:

$$\hat{y} \leftarrow \underset{v \in \text{values}(Y)}{\text{argmax}} \sum_{i=1}^{k} \delta(v, y^{(i)})$$

  - v = Yes. $\sum_{i=1}^{k} \delta(v, y^{(i)}) = 0 + 1 + 0 = 1$
  - v = No. $\sum_{i=1}^{k} \delta(v, y^{(i)}) = 1 + 0 + 1 = 2$ 

So, which class this new instance should be in?

How can we determine similarity/distance

- Suppose all features are continuous, where $x_f^{(i)}$ represents the f -th feature of $x^{(i)}$
  - Euclidean distance: $d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sqrt{\sum_f \left(x_f^{(i)} - x_f^{(j)}\right)^2}$
  - Manhattan distance: $d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sum_f \left|x_f^{(i)} - x_f^{(j)}\right|$

Recall the difference and similarity with L^p norm

More example

- Example: X = (Height, Weight, RunningSpeed) Y = SoccerPlayer?
  - D: in the table
  - New instance: <185, 91, 13.0>
  - Suppose that Euclidean distance is used.
  - Is this person a soccer player?

v1	v2	v3	y
182	87	11.3	No
189	92	12.3	Yes
178	79	10.6	Yes
183	90	12.7	No

Leave this as exercise for you.

New datum

185	91	13.0	

How to work with a mix of discrete/continuous features

- If we have a mix of discrete/continuous features:

$$d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sum_f \begin{cases} \left| x_f^{(i)} - x_f^{(j)} \right| & \text{if } f \text{ is continuous} \\ 1 - \delta\left(x_f^{(i)}, x_f^{(i)}\right) & \text{if } f \text{ is discrete} \end{cases}$$

- Typically want to apply to continuous features some type of normalization (values range 0 to 1) or standardization (values distributed according to standard normal)
- Many other possible distance functions we could use ...

Pre-processing – Standardisation of numeric features

- Given the training set D, determine the mean and stddev for feature x_i

$$\mu_i = \frac{1}{|D|}\sum_{d=1}^{|D|} x_i^{(d)} \qquad \sigma_i = \sqrt{\frac{1}{|D|}\sum_{d=1}^{|D|}\left(x_i^{(d)} - \mu_i\right)^2}$$

- Standardize each value of feature x_i as follows

$$\hat{x}_i^{(d)} = \frac{x_i^{(d)} - \mu_i}{\sigma_i}$$

- Do the same for test instances, using the same μ and σ derived from the *training* data

Confidence for k-NN classification (example)

- Classification steps are the same, recall $\hat{y} \leftarrow \underset{v \in values(Y)}{\operatorname{argmax}} \sum_{i=1}^{k} \delta(v, y^{(i)})$
- Given a class $\hat{y}$, we compute

$$acc\_dist = \sum_{i=1}^{k} \delta(\hat{y}, y^{(i)}) \cdot distance(\hat{y}, y^{(i)})$$

Accumulated distance to the supportive instances

- apply sigmoid function on the reciprocal of the accumulated distance

$$confidence = \frac{1}{1 + e^{-\frac{1}{acc\_dist}}}$$

Here, the confidences of all classes may not add up to 1

Softmax?

Speeding up k-NN

Issues

- Choosing k
  - Increasing k reduces variance, increases bias
- For high-dimensional space, problem that the nearest neighbor may not be very close at all!
- Memory-based technique. Must make a pass through the data for each classification. This can be prohibitive for large data sets.

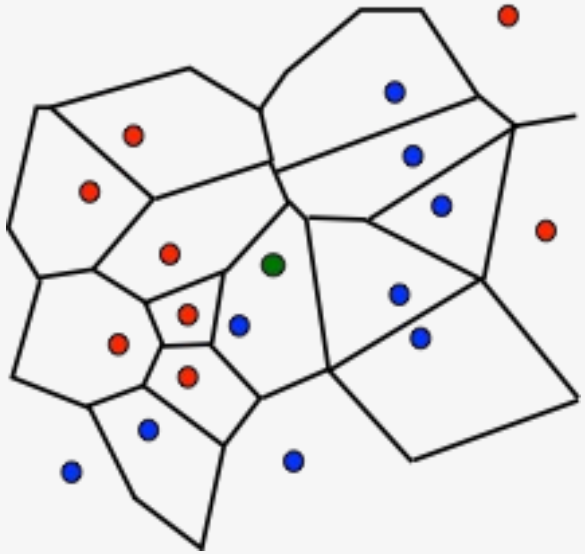
Nearest neighbour problem

- Given sample S = $((x_1,y_1),...,(x_m,y_m))$ and a test point x,
- It is to find the nearest k neighbours of x.

- Note: for the algorithms, dimensionality N, i.e., number of features, is crucial.

Efficient Indexing: N=2

- Algorithm
  - compute Voronoi diagram in O(m log m)
    - See algorithm in https://en.wikipedia.org/wiki/Fortune's_algorithm
  - use point location data structure to determine nearest neighbours
  - complexity: O(m) space, O(log m) time.



Efficient Indexing: N>2

- Voronoi diagram: size in $O(m^{N/2})$
- Linear algorithm (no pre-processing):
  - compute distance $||x - x_i||$ for all $i \in [1, m]$.
  - complexity of distance computation: $\Omega(N\ m)$.
  - no additional space needed.

k-NN is a “lazy” learning algorithm – does virtually nothing at training time

but classification/prediction time can be costly when the training set is large

Efficient Indexing: N>2

- Two general strategies for alleviating this weakness
  - don't retain every training instance (edited nearest neighbor)
  - pre-processing. Use a smart data structure to look up nearest neighbors (e.g. a k-d tree)

Edited instance-based learning

- Select a subset of the instances that still provide accurate classifications
- *Incremental deletion*

```
start with all training instances in memory
for each training instance (x^(i), y^(i))
    if other training instances provide correct classification for (x^(i), y^(i))
        delete it from the memory
```

Q1: Does ordering matter?

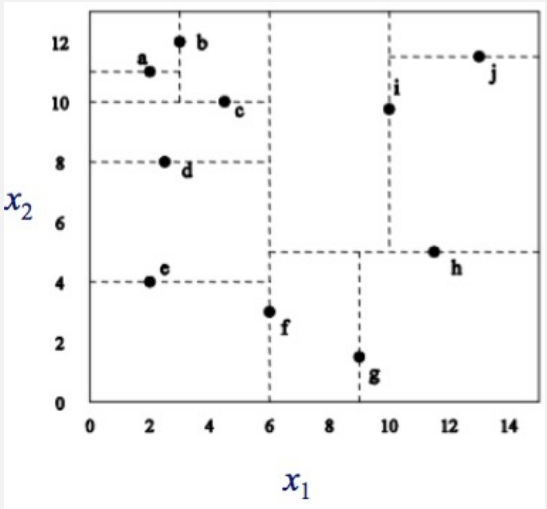
- *Incremental growth*

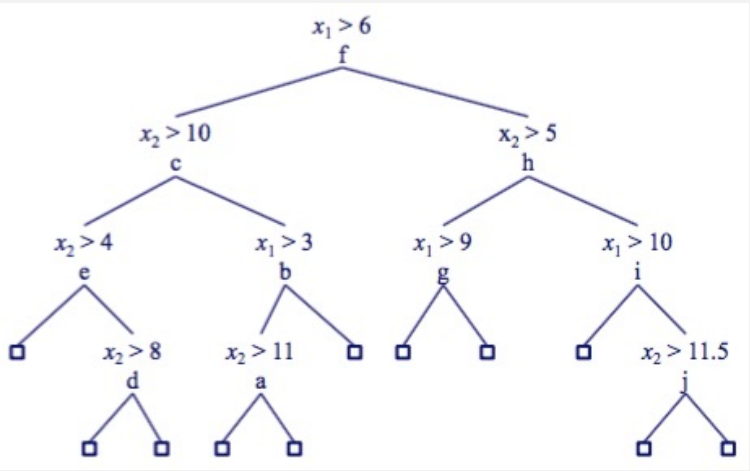
```
start with an empty memory
for each training instance (x^(i), y^(i))
    if other training instances in memory don't correctly classify (x^(i), y^(i))
        add it to the memory
```

Q2: If following the optimal ordering, do the two approaches produce the same subset of instances?

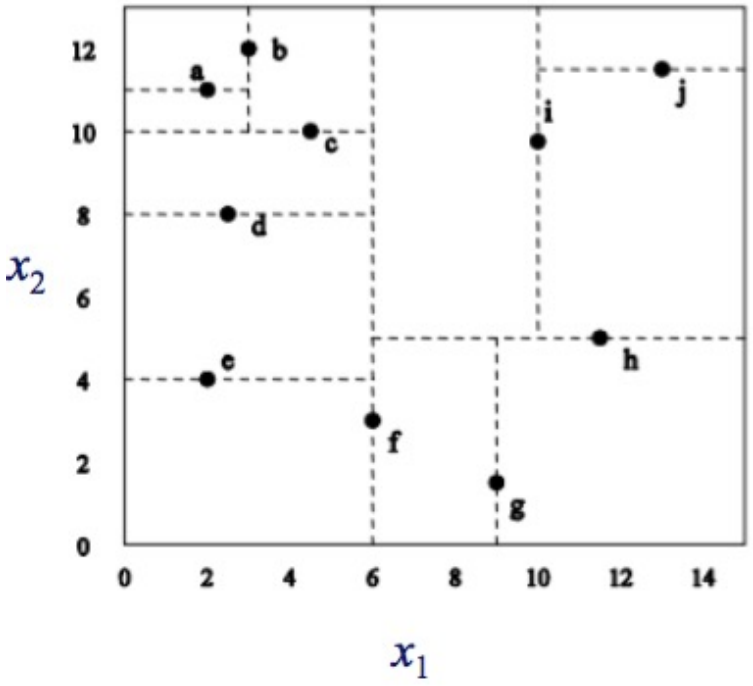
k-d trees

- A *k-d tree* is similar to a decision tree except that each internal node
  - stores one instance
  - splits on the median value of the feature having the highest variance





Construction of k-d tree



Determine a triple:

- the feature having the highest variance
- Median value of the feature
- Related data point.

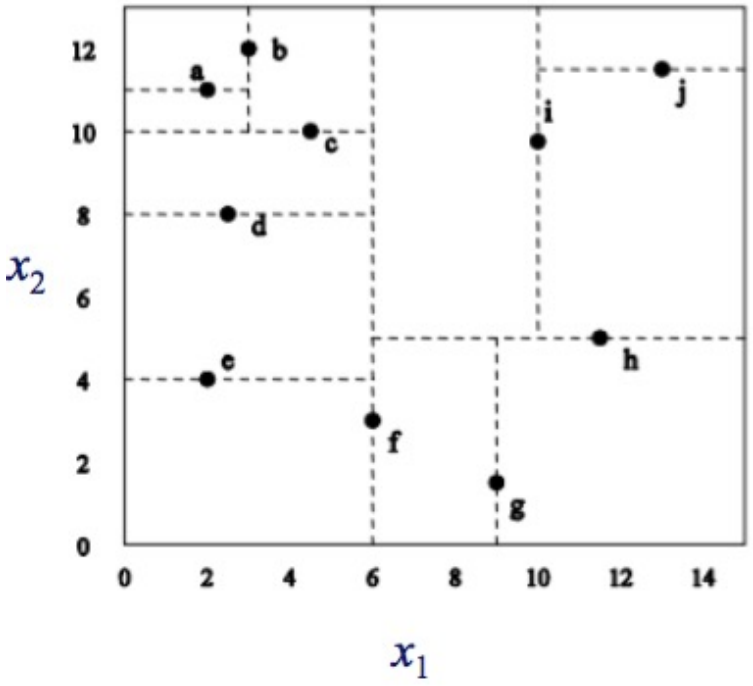
Example:

-- point f, $x_1 = 6$

$x_1>6$

f

Construction of k-d tree



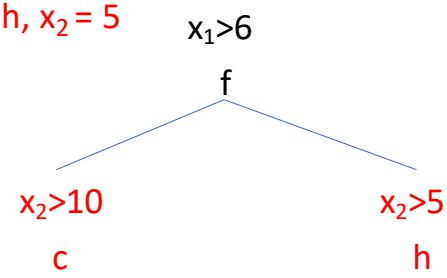
Determine a triple:

- the feature having the highest variance
- Median value of the feature
- Related data point.

Example:

-- point f, $x_1 = 6$

-- point c, $x_2 = 10$ and point h, $x_2 = 5$



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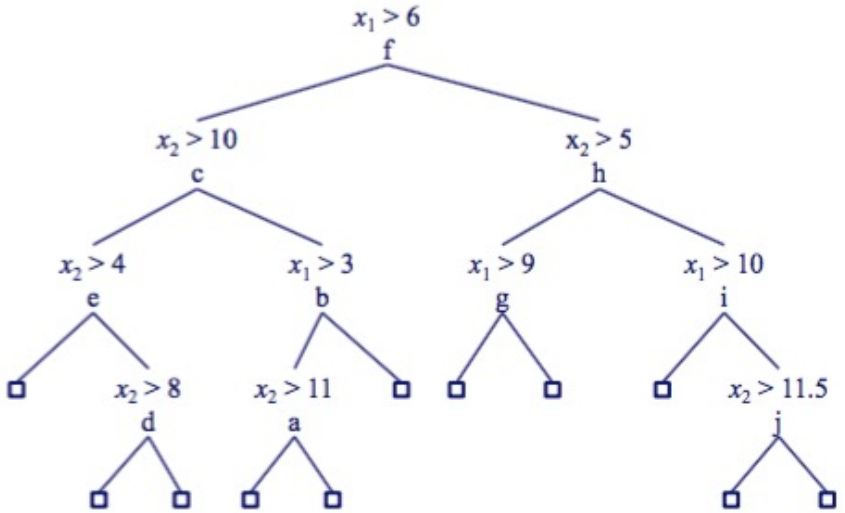
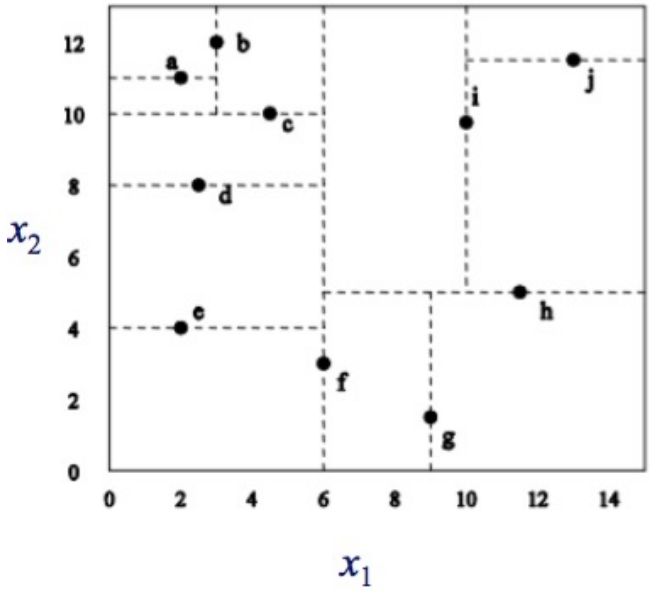




There can be other methods of constructing k-d trees, see e.g., https://en.wikipedia.org/wiki/K-d_tree#Nearest_neighbour_search

Finding nearest neighbors on a k-d tree

- use branch-and-bound search
- priority queue stores
  - nodes considered
  - lower bound on their distance to query instance
- lower bound given by distance using a single feature
- average case: $O(\log_2 m)$
- worst case: O(m) where m is the size of the training-set

Finding nearest neighbours in a k-d tree

```
NearestNeighbor(instance x^(q))
    PQ = { }                                    // minimizing priority queue
    best_dist = ∞                               // smallest distance seen so far
    PQ.push(root, 0)
    while PQ is not empty
        (node, bound) = PQ.pop();
        if (bound ≥ best_dist)
            return best_node.instance           // nearest neighbor found
        dist = distance(x^(q), node. instance)
        if (dist < best_dist)
            best_dist = dist
            best_node = node
        if (q[node.feature] – node.threshold > 0)
            PQ.push(node.left, x^(q)[node.feature] – node.threshold)
            PQ.push(node.right, 0)
        else
            PQ.push(node.left, 0)
            PQ.push(node.right, node. threshold - x^(q) [node.feature])
    return best_node. instance
```

Intuitively, for a pair (*node*,*bound*), *bound* represents the smallest guaranteed distance, i.e., greatest lower bound up to now, from the instance $x^{(q)}$ to the set of instances over which *node* is the selected one to split

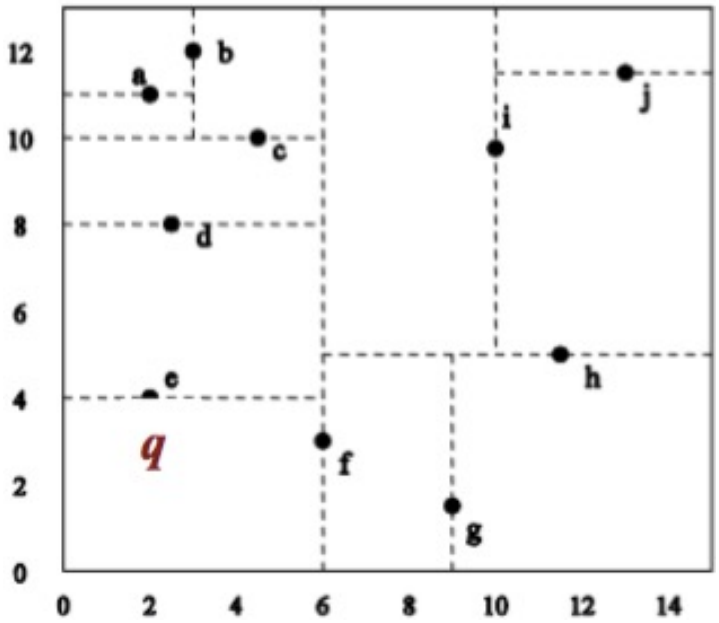
For example, the set of instances where *root* is the selected one to split over is the whole training set.

(root,0) means that at the beginning, the guaranteed smallest distance to the training set is 0

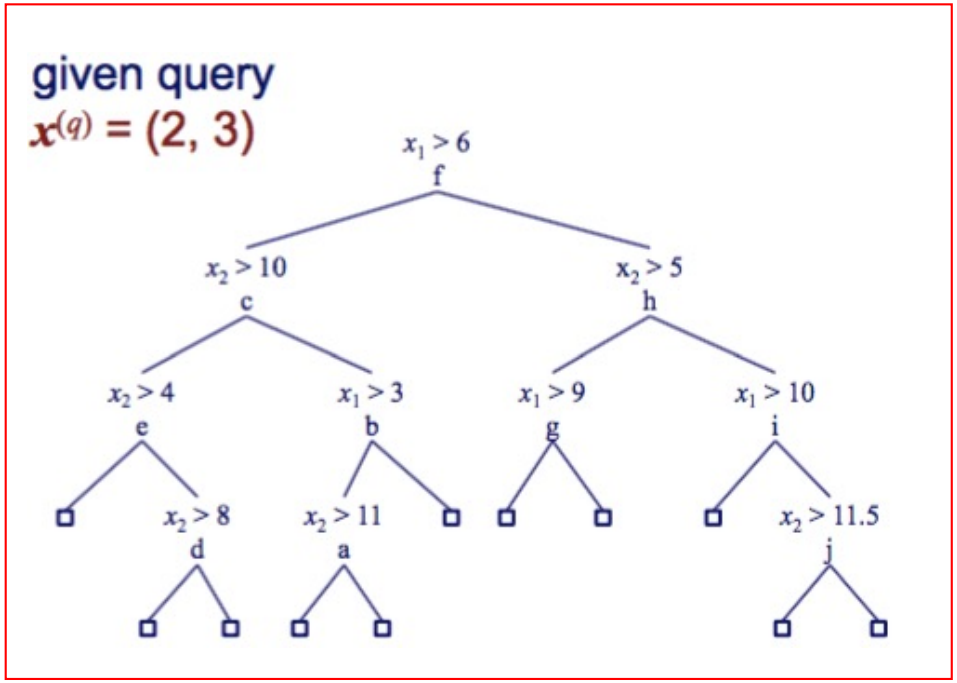
General idea: maintain a *best_dist* and a priority queue of *(node,bound)* pair, and terminate when *best_dist* becomes no greater than *bound*.

k-d tree example (Manhattan distance)

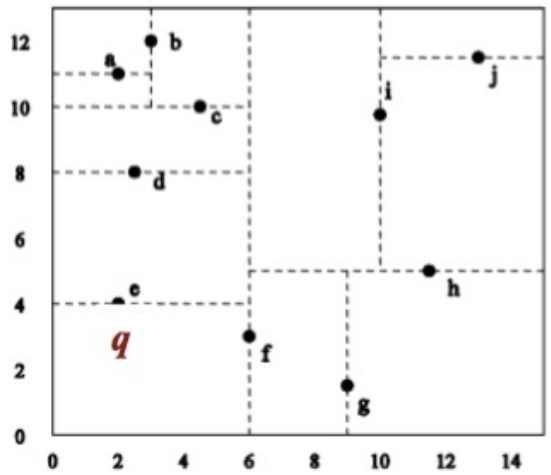
Can't see any more

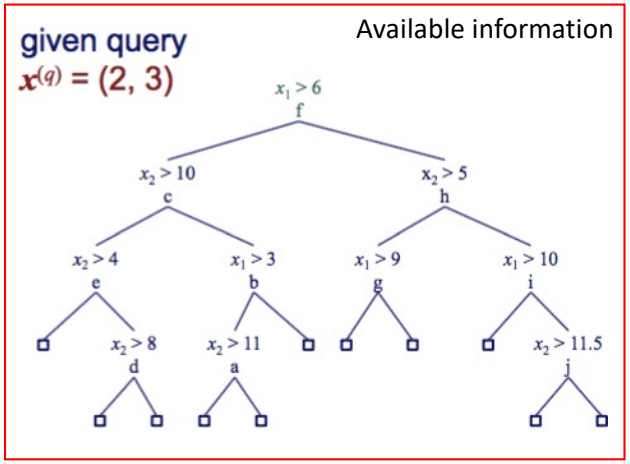


Available information



k-d tree example (Manhattan distance)



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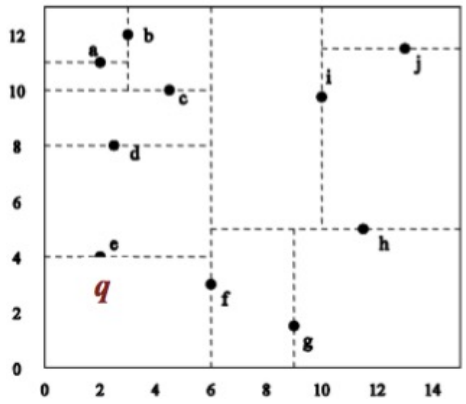
(node, bound) = PQ.pop();
if (bound ≥ best_dist)
        return best_node.instance
dist = distance(x^(q), node. instance)
if (dist < best_dist)
        best_dist = dist
        best_node = node
if (q[node.feature] – node.threshold > 0)
        PQ.push(node.left, x^(q)[node.featı
        PQ.push(node.right, 0)
else
        PQ.push(node.left, 0)
        PQ.push(node.right, node. thresh
```

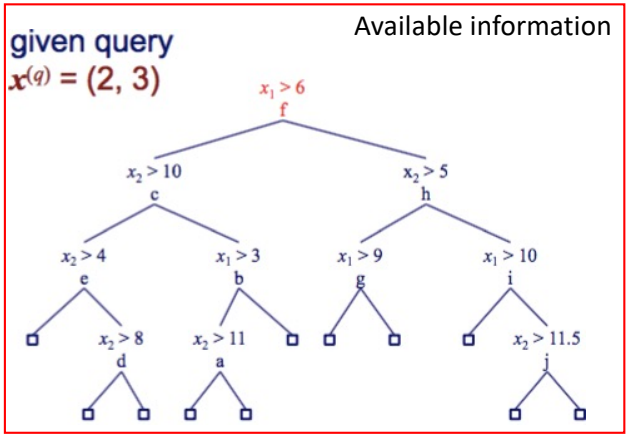
distance	best distance	best node	priority queue
	∞		(f, 0)

Initialise *best_dist* as infinity

Push in the root node

k-d tree example (Manhattan distance)





	distance	best distance	best node	priority queue
		∞		(f, 0)
pop f	4.0	4.0	f	

The distance between *q* and *f*

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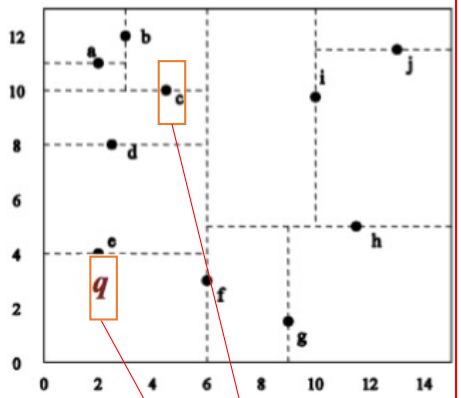
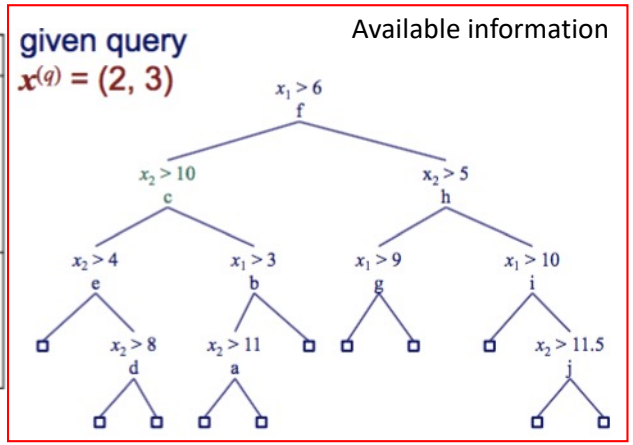
k-d tree example (Manhattan distance)



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```

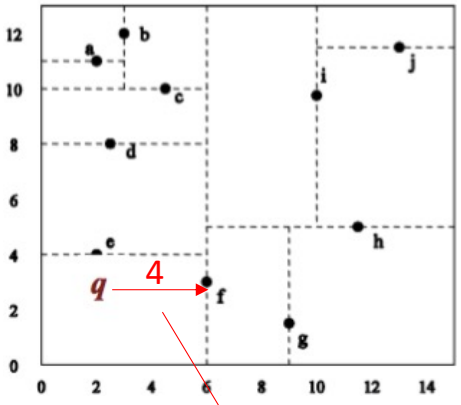
pop f

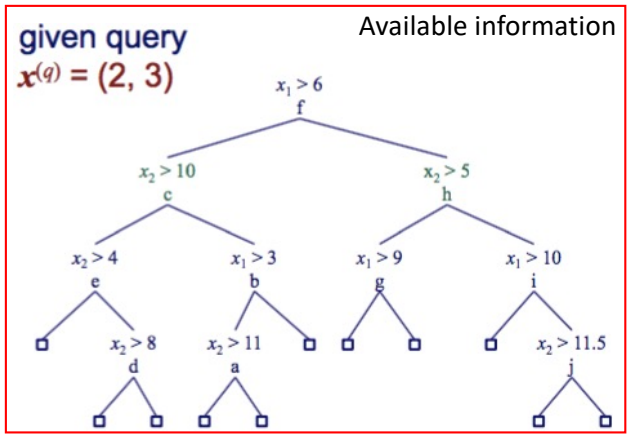
distance	best distance	best node	priority queue
	∞		(f, 0)
4.0	4.0	f	(c, 0)

Because *q* and *c* are on the same side of *f*

Why *0*?

k-d tree example (Manhattan distance)



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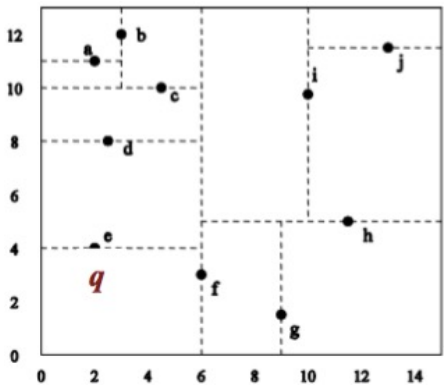
```

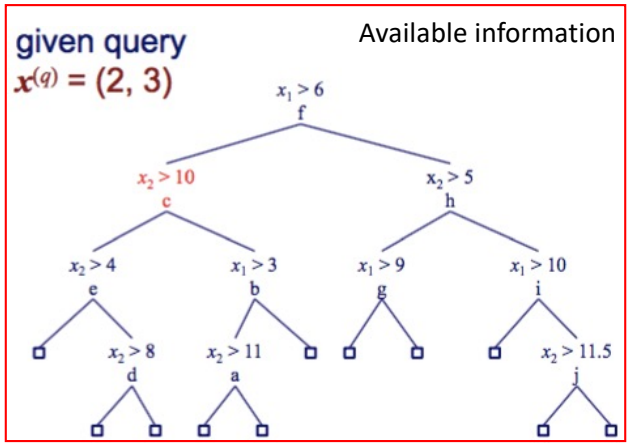
pop f

distance	best distance	best node	priority queue
	∞		(f, 0)
4.0	4.0	f	(c, 0) (h, 4)

Because the shortest distance from *q* to the other side of *f* is 4 ← Why 4?

k-d tree example (Manhattan distance)



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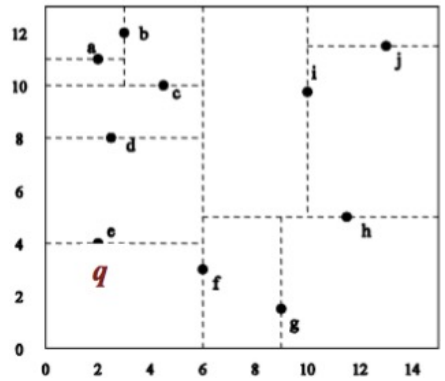
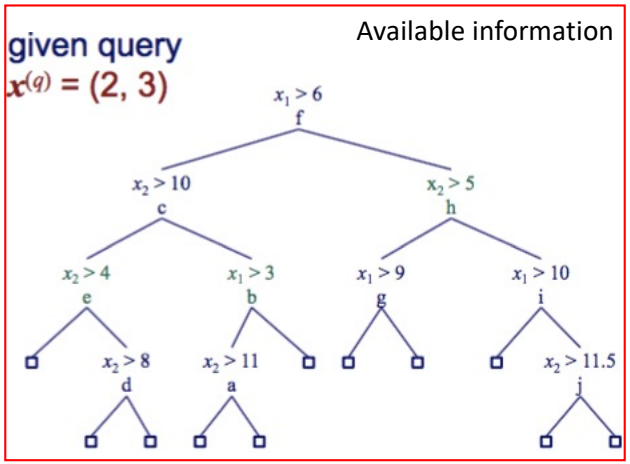
```

	distance	best distance	best node	priority queue
		∞		(f, 0)
pop f	4.0	4.0	f	(c, 0) (h, 4)
pop c	10.0	4.0	f	

The distance between *q* and *c*

k-d tree example (Manhattan distance)






```
(node, bound) = PQ.pop();
if (bound ≥ best_dist)
        return best_node.instance
dist = distance(x^(q), node. instance)
if (dist < best_dist)
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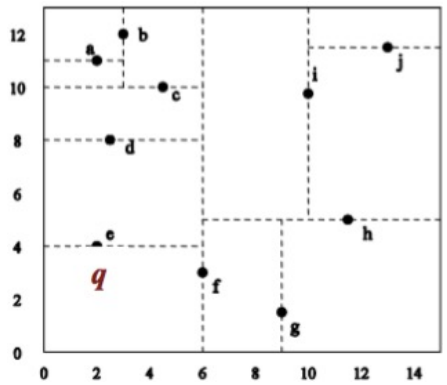
        best_node = node
if (q[node.feature] – node.threshold > 0)
        PQ.push(node.left, x^(q)[node.featı
        PQ.push(node.right, 0)
else
        PQ.push(node.left, 0)
        PQ.push(node.right, node. thresh
```

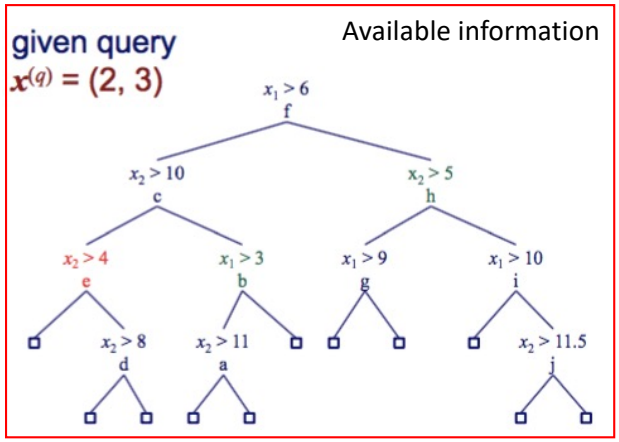
	distance	best distance	best node	priority queue
		∞		(f, 0)
pop f	4.0	4.0	f	(c, 0) (h, 4)
pop c	10.0	4.0	f	(e, 0) (h, 4) (b, 7)

e and *q* are at the same side of *c*

b and *q* are at the different side of *c*, and 7 is the shortest distance from *q* to the boundary

k-d tree example (Manhattan distance)



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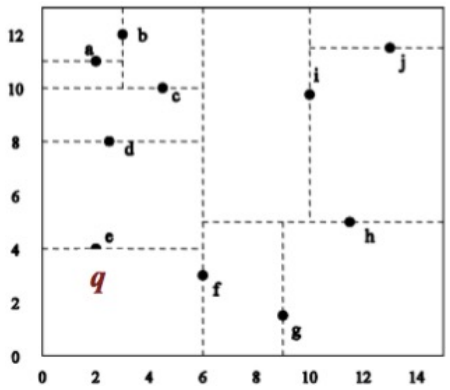
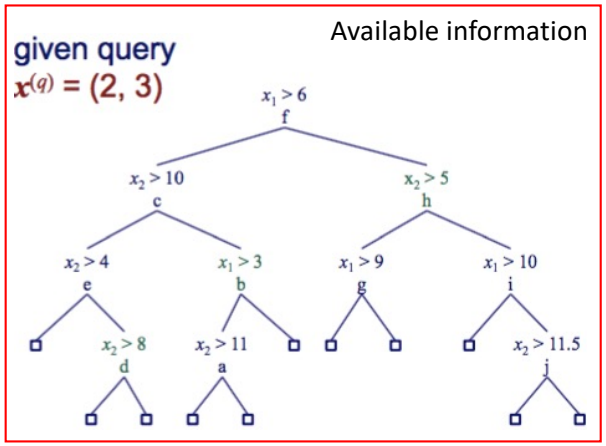
pop c	10.0	4.0	f	(e, 0) (h, 4) (b, 7)
pop e	1.0	1.0	e	

The distance between *q* and *e*

Now we can update best_dist because 1<4

k-d tree example (Manhattan distance)



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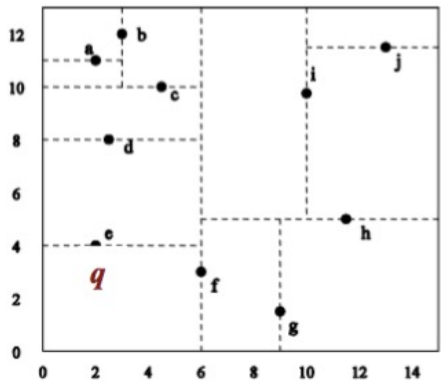
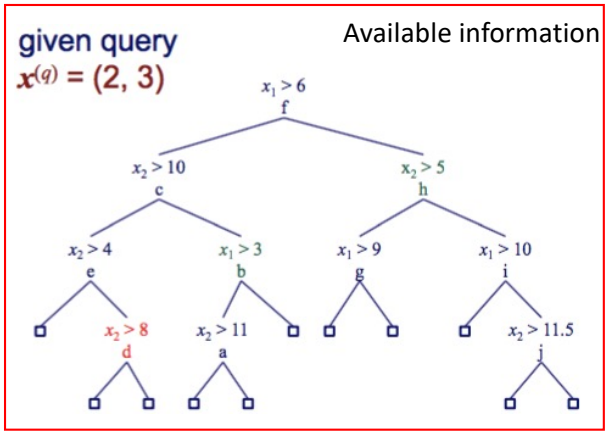
pop e	1.0	1.0	e	(d, 1) (h, 4) (b, 7)

d and *q* are at the different side of *e*, and 1 is the shortest distance from *q* to the boundary

k-d tree example (Manhattan distance)



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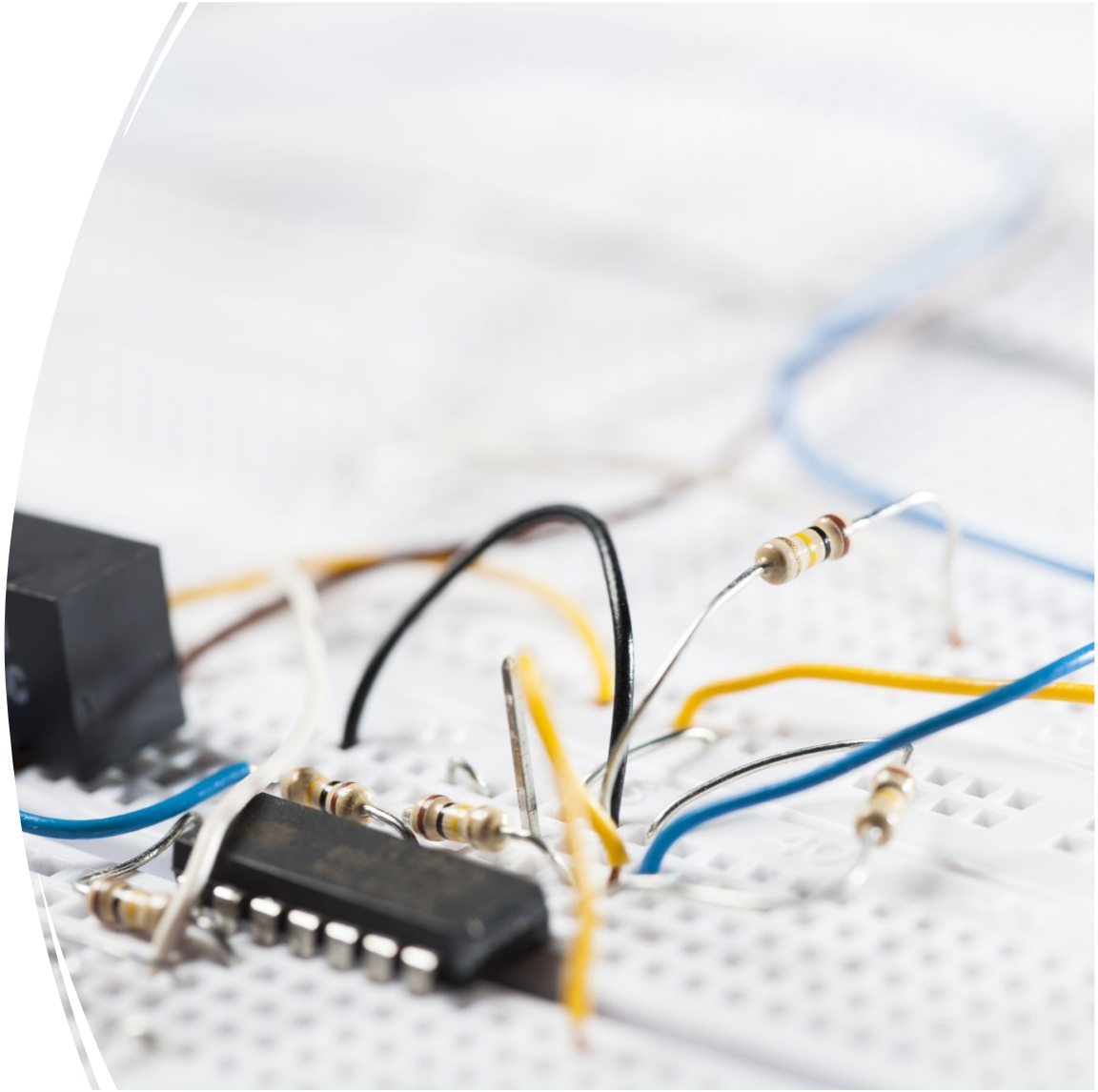
```

	distance	best distance	best node	priority queue
		∞		(f, 0)
pop f	4.0	4.0	f	(c, 0) (h, 4)
pop c	10.0	4.0	f	(e, 0) (h, 4) (b, 7)
pop e	1.0	1.0	e	(d, 1) (h, 4) (b, 7)
pop d	return e			

Now we have *best_dist = bound*, return the node *e*

Extended Materials: Voronoi Diagram Generation

- https://en.wikipedia.org/wiki/Voronoi_diagram
- https://courses.cs.washington.edu/courses/cse326/00wi/projects/voronoi.html



Variants of k-NN

k-nearest-neighbor *regression*

- learning stage
  - given a training set $(\mathbf{x}^{(1)}, y^{(1)}) \ldots (\mathbf{x}^{(m)}, y^{(m)})$, do nothing
    - (it's sometimes called a *lazy learner*)

- classification stage
  - **given**: an instance $x^{(q)}$ to classify
  - find the k training-set instances $(\mathbf{x}^{(1)}, y^{(1)}) \ldots (\mathbf{x}^{(k)}, y^{(k)})$ that are most similar to $x^{(q)}$
  - return the value

$$\hat{y} \leftarrow \frac{1}{k} \sum_{i=1}^{k} y^{(i)}$$

Average over neighbours' values

Distance-weighted nearest neighbor

- We can have instances contribute to a prediction according to their distance from $x^{(q)}$
- classification:

$$\hat{y} \leftarrow \underset{v \in values(Y)}{\operatorname{argmax}} \sum_{i=1}^{k} w_i \, \delta(v, y^{(i)})$$

$$w_i = \frac{1}{d(x^{(q)}, x^{(i)})^2}$$

Intuition: instances closer to the current one is more important.

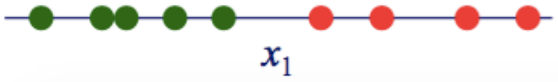
reciprocal of the distance

- regression:

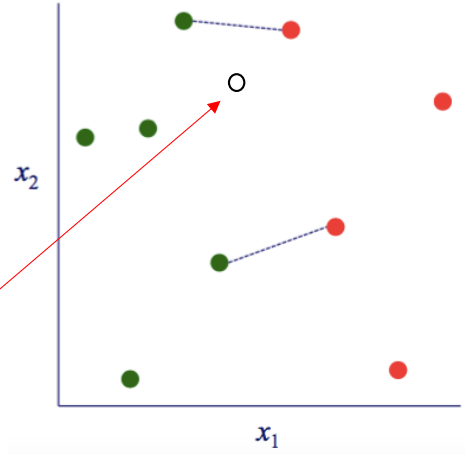
$$\hat{y} \leftarrow \frac{\sum_{i=1}^{k} w_i \, y^{(i)}}{\sum_{i=1}^{k} w_i}$$

Irrelevant features in instance-based learning

here's a case in which there is one relevant feature x_1 and a 1-NN rule classifies each instance correctly



consider the effect of an irrelevant feature x_2 on distances and nearest neighbors



Can you find a point (a,b) which is red, if classified only according to feature x1, and is green, if classified according to both features?

Locally weighted regression

- one way around this limitation is to weight features differently
- *locally weighted regression* is one nearest-neighbor variant that does this

- prediction task
  - **given**: an instance $x^{(q)}$ to make a prediction for
  - find the k training-set instances $(\mathbf{x}^{(1)}, y^{(1)}) \ldots (\mathbf{x}^{(k)}, y^{(k)})$ that are most similar to $x^{(q)}$
  - return the value $f(x^{(q)})$

What's function f ?

Locally weighted regression

- Determining function f
  - Assume that f is a linear function over the features, i.e.,

$$f(x^{(i)}) = w_0 + w_1 x_1^{(i)} + w_2 x_2^{(i)} + \ldots + w_n x_n^{(i)}$$

  - find the weights w_i for each $x^{(q)}$ by

$$arg \min_{w_0, w_1, \ldots, w_n} \sum_{i=1}^{k} (f(x^{(i)}) - y^{(i)})^2$$

can do this using gradient descent (to be introduced soon)

  - After obtaining weights, for $x^{(q)}$, we have $f(\mathbf{x}^{(q)}) = w_0 + w_1 x_1^{(q)} + w_2 x_2^{(q)} + \ldots + w_n x_n^{(q)}$

Discussions

Strengths of instance-based learning

- simple to implement
- “training” is very efficient
- adapts well to on-line learning
- robust to noisy training data (when k > 1)
- often works well in practice

Limitations of instance-based learning

- sensitive to range of feature values
- sensitive to irrelevant and correlated features, although ...
  - there are variants (such as locally weighted regression) that learn weights for different features
- classification/prediction can be inefficient, although …
  - edited methods and k-d trees can help alleviate this weakness
- doesn’t provide much insight into problem domain because there is no explicit model