Foundations of Machine Learning
CentraleSupélec Paris — Fall 2016

7. Nearest neighbors

Chloé-Agathe Azencott
Centre for Computational Biology, Mines ParisTech
chloe-agathe.azencott@mines-paristech.fr

Inserm
Institut national
de la santé et de la recherche médicale

institutCurie

MINES
ParisTech

Practical matters

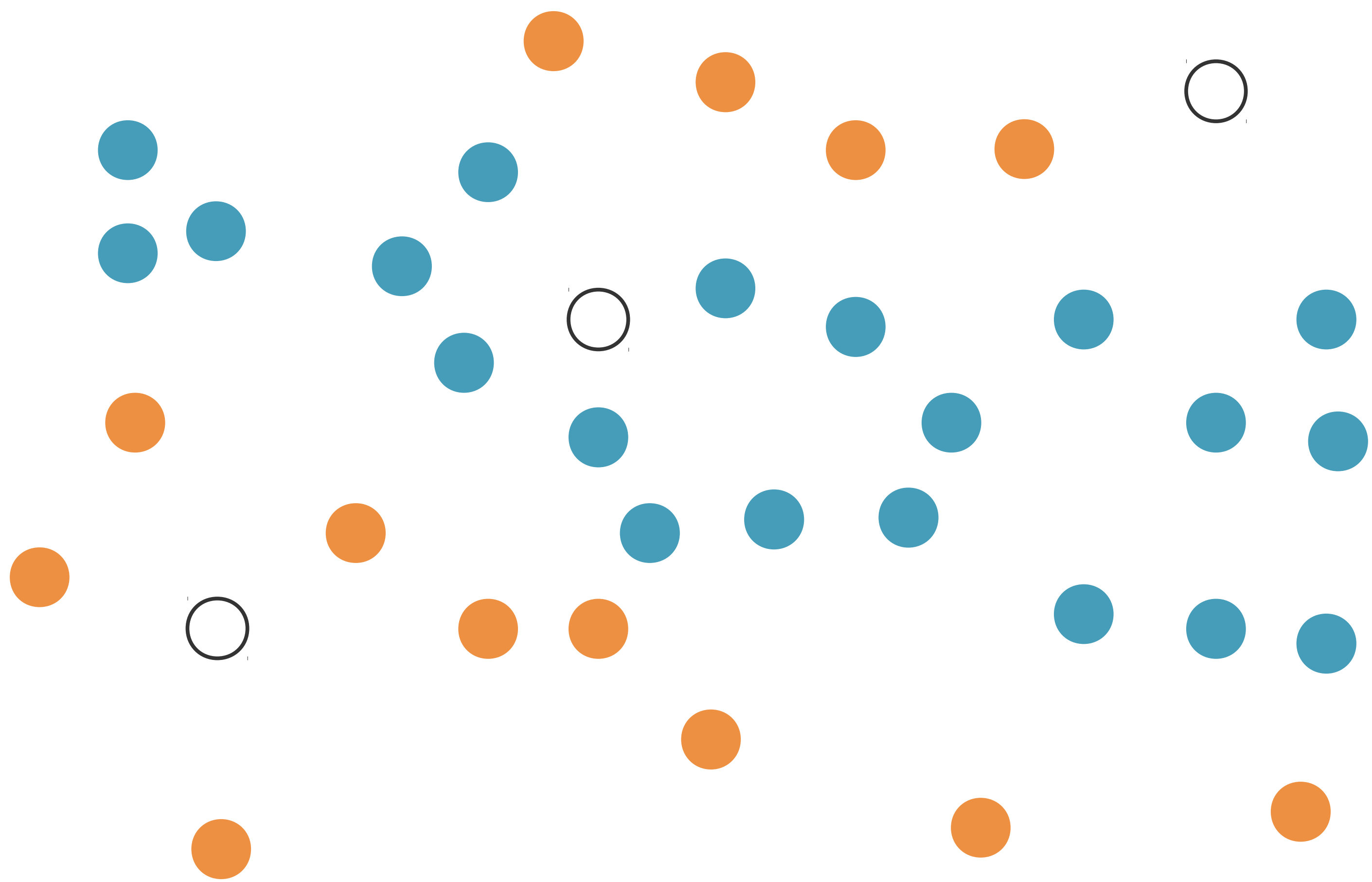
- **Homework** solutions
- **Kaggle project**
  - Get started early
  - You can do as many submissions as you want (! daily limit)
  - Submissions that will count towards your grade:
    - Last 3 submissions
    - Submissions I asked for, i.e. your best
      - linreg
      - regul_linreg
      - knn
      - trees
      - svm.

Learning objectives

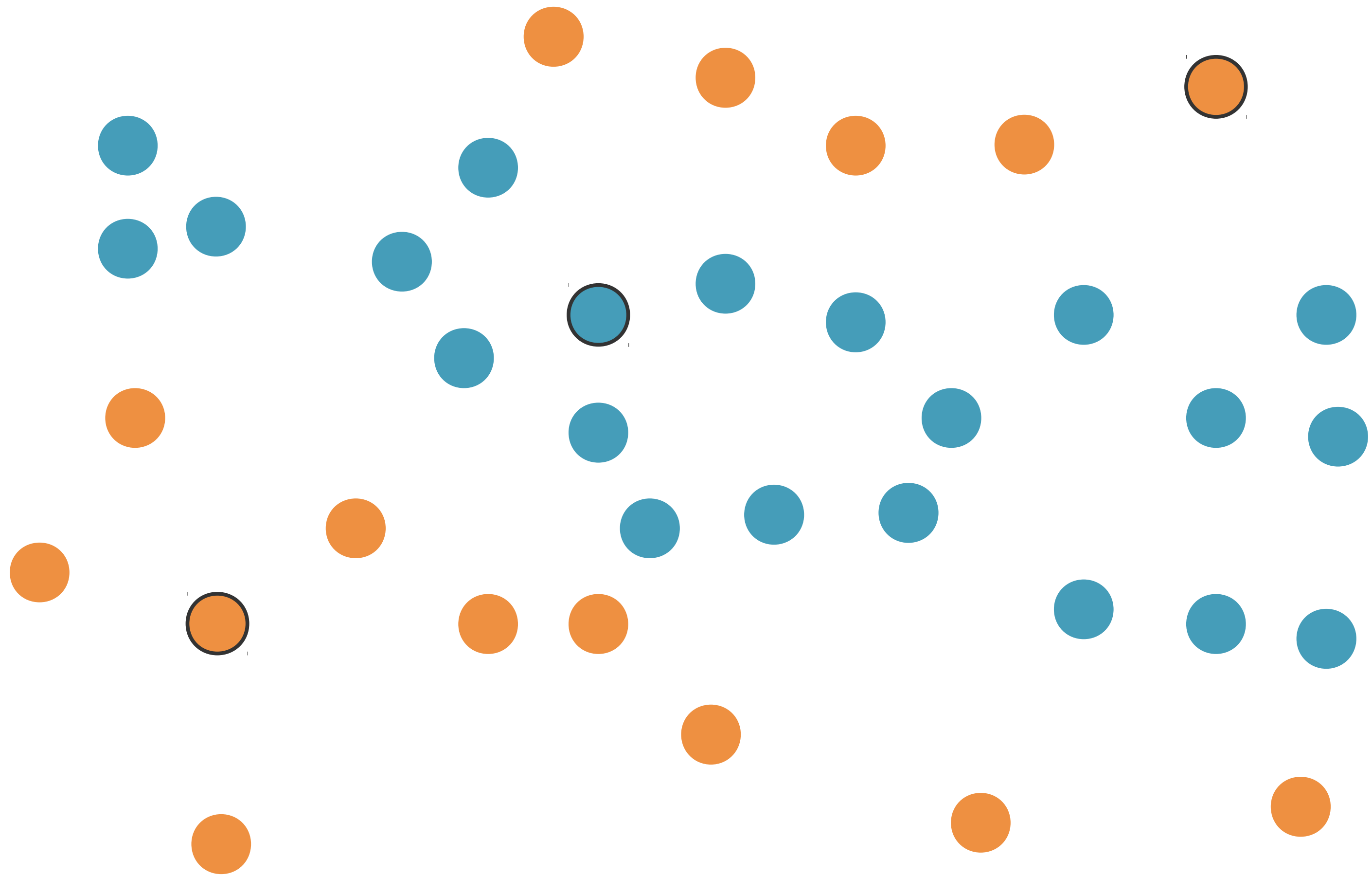
- Implement the **nearest-neighbor** and **k-nearest-neighbors** algorithms.
- Compute **distances** between **real-valued vectors** as well as objects represented by **categorical features**.
- Define the **decision boundary** of the nearest-neighbor algorithm.
- Explain why kNN might not work well in **high dimension**.

Nearest neighbors

- **How would you color the blank circles?**

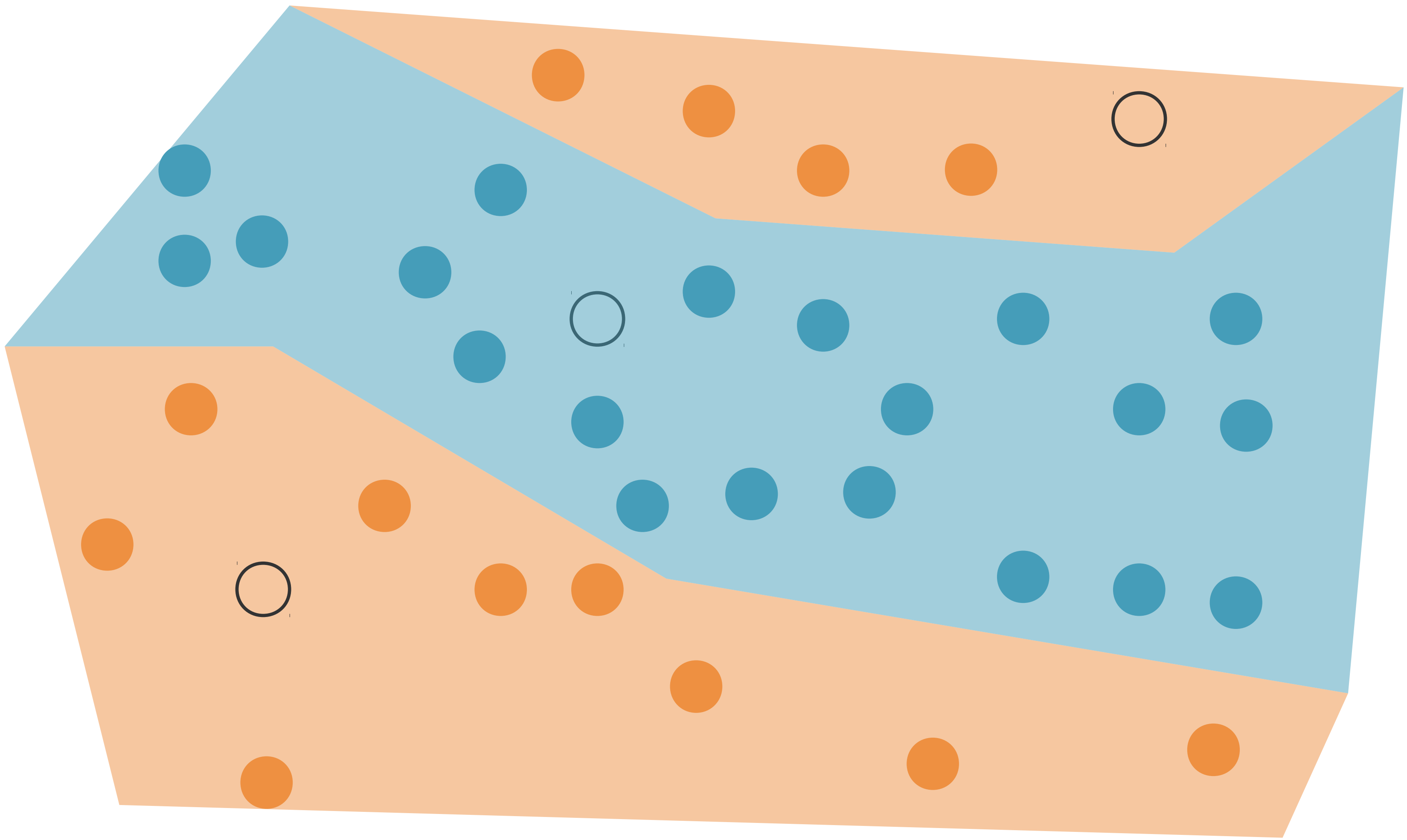


- **How would you color the blank circles?**



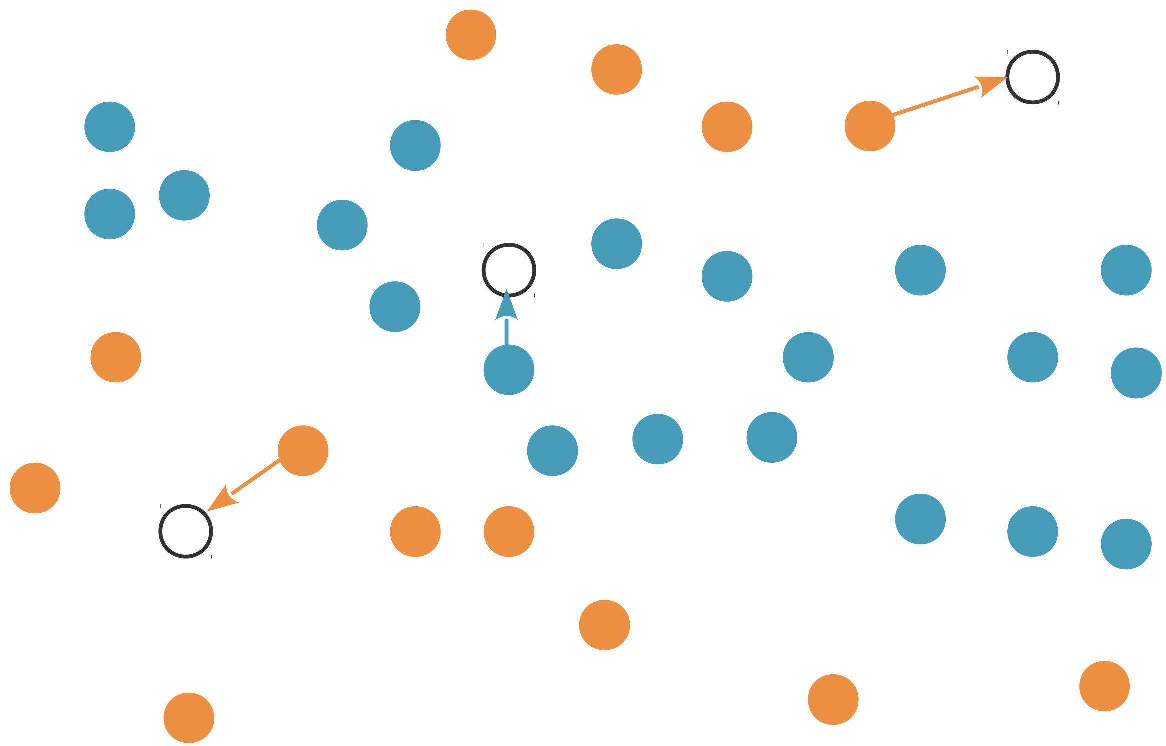
Partitioning the space

The training data partitions the entire space



Nearest neighbor

- **Learning:**
  - Store all the training examples
- **Prediction**:
  - For **x**: the label of the training example closest to it



k nearest neighbors

- **Learning:**
  - Store all the training examples
- **Prediction:**
  - Find the k training examples closest to **x**
  - **Classification?**

k nearest neighbors

- **Learning:**
  - Store all the training examples
- **Prediction:**
  - Find the k training examples closest to **x**
  - **Classification**

    Majority vote: Predict the class of the most frequent label among the k neighbors.

k nearest neighbors

- **Learning:**
  - Store all the training examples
- **Prediction:**
  - Find the k training examples closest to x
  - **Classification**

    Majority vote: Predict the class of the most frequent label among the k neighbors.
  - **Regression?**

k nearest neighbors

- **Learning:**
  - Store all the training examples
- **Prediction:**
  - Find the k training examples closest to x
  - **Classification**

    Majority vote: Predict the class of the most frequent label among the k neighbors.
  - **Regression**

    Predict the average of the labels of the k neighbors.

Choice of k

- **Small k:** noisy

  The idea behind using more than 1 neighbor is to average out the noise

- **Large k:** computationally intensive

  Also, what happens if k = n?

Choice of k

- **Small k:** noisy

  The idea behind using more than 1 neighbor is to average out the noise

- **Large k:** computationally intensive

  If k=n, then we predict

  - for classification: the majority class
  - for regression: the average value

- Set k by **cross-validation**
- Heuristic: **$k \approx \sqrt{n}$**

Non-parametric learning

Non-parametric learning algorithm:

- **the complexity of the decision function grows with the number of data points.**
- contrast with linear regression (≈ as many parameters as features).
- Usually: decision function is expressed directly in terms of the training examples.
- Examples:
  - kNN (this chapter)
  - tree-based methods (Chap. 8)
  - SVM (Chap. 9)
  - neural networks (Chap. 10), in some cases.

Instance-based learning

- **Learning:**
  - Storing training instances.
- **Predicting:**
  - Compute the label for a new instance based on its **similarity** with the stored instances.

- Also called **lazy learning.**
- Similar to **case-based reasoning**
  - Doctors treating a patient based on how patients with similar symptoms were treated,
  - Judges ruling court cases based on legal precedent.

Instance-based learning

- **Learning:**
  - Storing training instances.
- **Predicting:**
  - Compute the label for a new instance based on its **similarity** with the stored instances.

where the magic happens!

- Also called **lazy learning.**
- Similar to **case-based reasoning**
  - Doctors treating a patient based on how patients with similar symptoms were treated,
  - Judges ruling court cases based on legal precedent.

Computing distances & similarities

Distances between instances

- **Distance**

$$d : \mathcal{X} \to \mathbb{R}_+$$

Distances between instances

- **Distance**

$$d : \mathcal{X} \to \mathbb{R}_+$$

1. $d(\boldsymbol{x}, \boldsymbol{x}) = 0$
2. $d(\boldsymbol{x}, \boldsymbol{z}) = d(\boldsymbol{z}, \boldsymbol{x})$
3. $d(\boldsymbol{x}, \boldsymbol{z}) \leq d(\boldsymbol{x}, \boldsymbol{u}) + d(\boldsymbol{u}, \boldsymbol{x})$

Distances between instances

$\boldsymbol{x} \in \mathbb{R}^p$

- **Euclidean distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_2 = \sqrt{\sum_{j=1}^{p} \left(x_j^1 - x_j^2\right)^2}$$

Distances between instances

$\boldsymbol{x} \in \mathbb{R}^p$

- **Euclidean distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_2 = \sqrt{\sum_{j=1}^{p} \left(x_j^1 - x_j^2\right)^2}$$

- **Manhattan distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_1 = \sum_{j=1}^{p} |x_j^1 - x_j^2|$$

Why is this called the Manhattan distance?

Distances between instances

$$\boldsymbol{x} \in \mathbb{R}^p$$

- **Euclidean distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_2 = \sqrt{\sum_{j=1}^{p} \left(x_j^1 - x_j^2\right)^2}$$

- **Manhattan distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_1 = \sum_{j=1}^{p} |x_j^1 - x_j^2|$$

- **Lq-norm**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_q = \left(\sum_{j=1}^{p} |x_j^1 - x_j^2|^q\right)^{1/q}$$

  - L1 = Manhattan.
  - L2 = Euclidean.
  - **What's L_∞?**

Distances between instances

$$\boldsymbol{x} \in \mathbb{R}^p$$

- **Euclidean distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_2 = \sqrt{\sum_{j=1}^{p} \left(x_j^1 - x_j^2\right)^2}$$

- **Manhattan distance**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_1 = \sum_{j=1}^{p} |x_j^1 - x_j^2|$$

- **Lq-norm**

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = ||\boldsymbol{x}^1 - \boldsymbol{x}^2||_q = \left(\sum_{j=1}^{p} |x_j^1 - x_j^2|^q\right)^{1/q}$$

  - L1 = Manhattan.
  - L2 = Euclidean.
  - **What's L_∞?**

$$L_\infty = \max_j(|x_j^1 - x_j^2|)$$

Similarity between instances

$$s = \frac{1}{1+d}$$

- Pearson's correlation

$$\rho(\boldsymbol{x}, \boldsymbol{z}) = \frac{\sum_{j=1}^{p} (x_j - \bar{x})(z_j - \bar{z})}{\sqrt{\sum_{j=1}^{p} (x_j - \bar{x})^2} \sqrt{\sum_{j=1}^{p} (z_j - \bar{z})^2}}$$

$$\bar{x} = \frac{1}{p} \sum_{j=1}^{p} x_j$$

- Assuming the data is centered

$$\rho(\boldsymbol{x}, \boldsymbol{z}) = \frac{\sum_{j=1}^{p} x_j z_j}{\sqrt{\sum_{j=1}^{p} x_j^2} \sqrt{\sum_{j=1}^{p} z_j^2}}$$

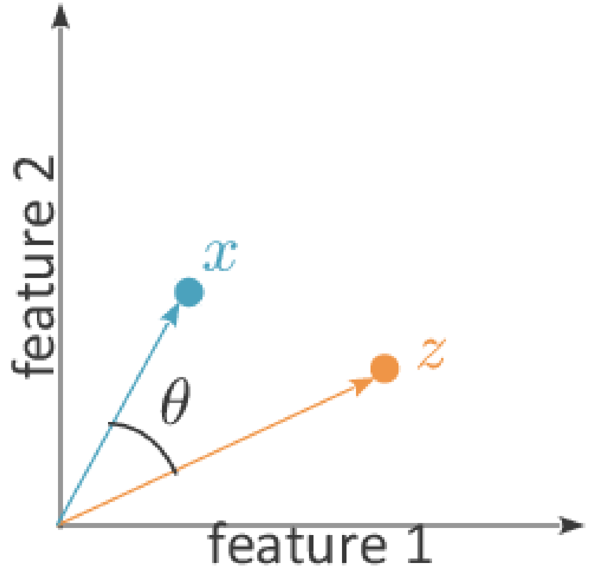
Geometric interpretation?

Similarity between instances

- Pearson's correlation (centered data)

$$\rho(\boldsymbol{x}, \boldsymbol{z}) = \frac{\sum_{j=1}^{p} x_j z_j}{\sqrt{\sum_{j=1}^{p} x_j^2}\sqrt{\sum_{j=1}^{p} z_j^2}} = \frac{\langle \boldsymbol{x}, \boldsymbol{z} \rangle}{||\boldsymbol{x}||.||\boldsymbol{z}||} = \cos\theta$$

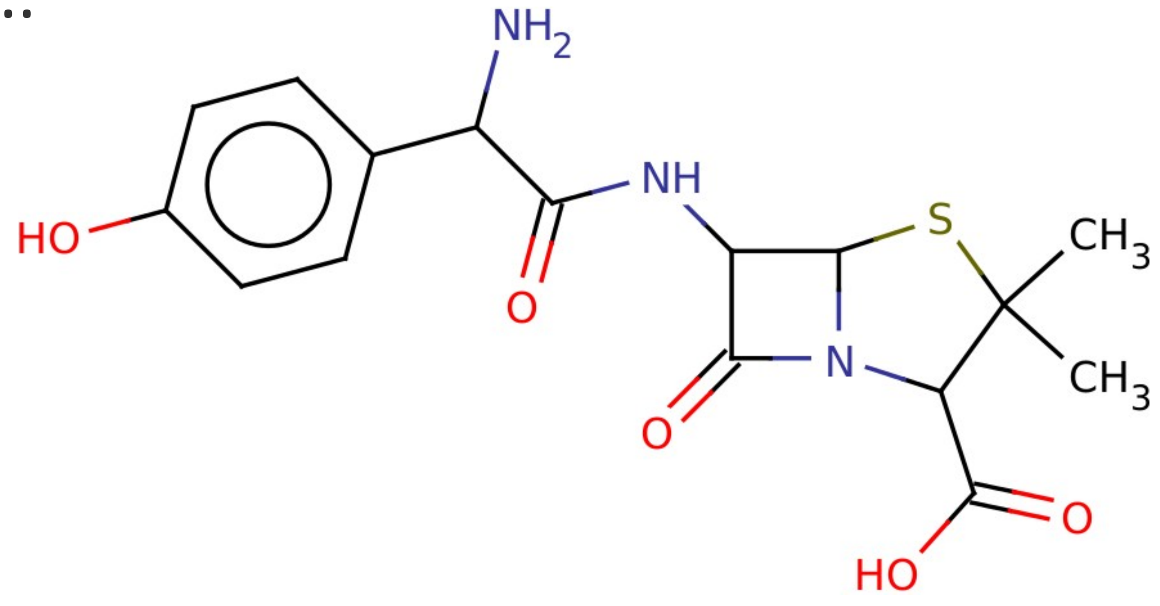
- **Cosine similarity:** the dot product can be used to measure similarities.



Categorical features

- Represent object as the list of **presence/absence** (or counts) of **features that appear in it.**
- **Example**: small molecules

  features = atoms and bonds of a certain type
  - C, H, S, O, N...
  - O-H, O=C, C-N....



Binary representation

0	1	1	0	0	1	0	0	0	1	0	1	0	0	1

no occurrence of the 1st feature

1+ occurrences of the 10th feature

- **Hamming distance**

  Number of bits that are different

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = \sum_{j=1}^{p} (x_j^1 \text{ XOR } x_j^2)$$

Equivalent to?

Binary representation

0	1	1	0	0	1	0	0	0	1	0	1	0	0	1

no occurrence of the 1st feature

1+ occurrences of the 10th feature

- **Hamming distance**

  Number of bits that are different

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = \sum_{j=1}^{p} (x_j^1 \text{ XOR } x_j^2)$$

  Equivalent to

$$d(\boldsymbol{x}^1, \boldsymbol{x}^2) = \sum_{j=1}^{p} |x_j^1 - x_j^2| = \sum_{j=1}^{p} (x_j^1 - x_j^2)^2$$

Binary representation

0	1	1	0	0	1	0	0	0	1	0	1	0	0	1

- **Tanimoto similarity**

  Number of shared features (normalized)

$$s(\boldsymbol{x}^1, \boldsymbol{x}^2) = \frac{\sum_{j=1}^{p} (x_j^1 \text{ AND } x_j^2)}{\sum_{j=1}^{p} (x_j^1 \text{ OR } x_j^2)}$$

Counts representation

0	1	2	0	0	1	0	0	0	4	0	1	0	0	7

no occurrence
of the 1st feature

occurrences
of the 10th feature

- **MinMax similarity**

  Number of shared features (normalized)

$$s(\boldsymbol{x}^1, \boldsymbol{x}^2) = \frac{\sum_{j=1}^{p} \min(x_j^1, x_j^2)}{\sum_{j=1}^{p} \max(x_j^1, x_j^2)}$$

  If x is binary, MinMax and Tanimoto are equivalent

$$s(\boldsymbol{x}^1, \boldsymbol{x}^2) = \frac{\sum_{j=1}^{p} (x_j^1 \text{ AND } x_j^2)}{\sum_{j=1}^{p} (x_j^1 \text{ OR } x_j^2)}$$

Categorical features

- Features

- **Compute the Hamming distance and Tanimoto and MinMax similarities between these objects:**

Categorical features

- Features

- **Compute the Hamming distance and Tanimoto and MinMax similarities between these objects:**

100011010110
300011010120

111011011110
211021011120

111011010100
311011010100

Categorical features

- `A = 100011010110 / 300011010120`
- `B = 111011011110 / 211021011120`
- `C = 111011010100 / 311011010100`

- **Hamming distance**

  d(A, B) = 3 d(A, C) = 3 d(B, C) = 2

- **Tanimoto similarity**

  s(A, B) = 6/9 = 0.67 s(A, C) = 5/8 = 0.63 s(B, C) = 7/9 = 0.78

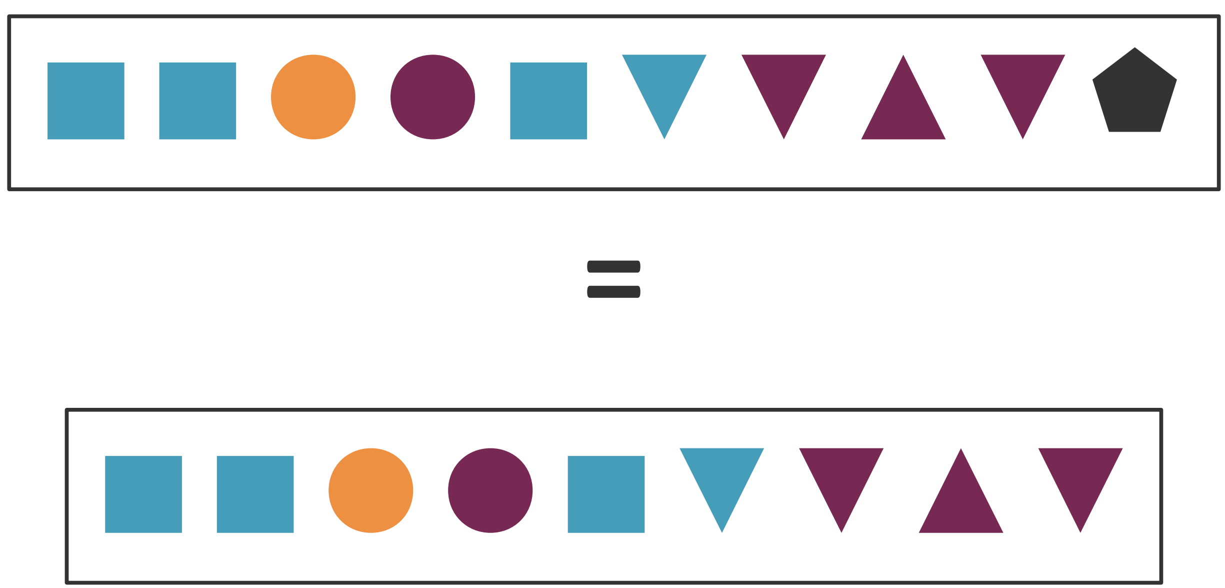
- **MinMax similarity**

  s(A, B) = 8/13 = 0.62 s(A, C) = 7/11 = 0.64 s(B, C) = 8/13 = 0.62

Categorical features

- Features

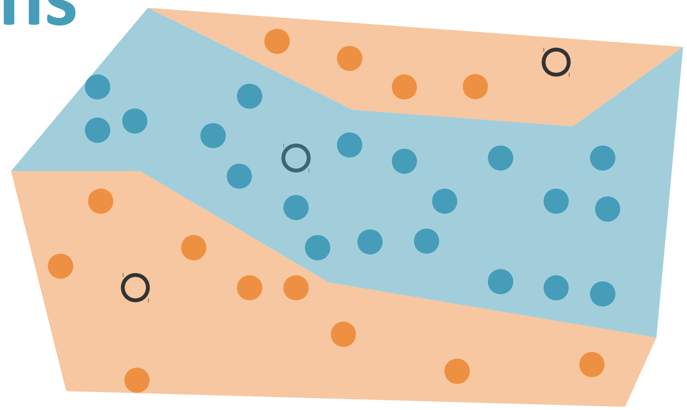
- When new data has unknown features: ignore them.



Back to nearest neighbors

Advantages of kNN

- Training is very fast
  - Just store the training examples.
  - Can use smart indexing procedures to speed-up testing (slower training).
- Keeps the training data
  - Useful if we want to do something else with it.
- Rather robust to noisy data (averaging k votes)
- Can learn complex functions



Drawbacks of kNN

- **Memory** requirements
- Prediction can be **slow.**
  - **What is the complexity of labeling 1 new data point?**

Drawbacks of kNN

- **Memory** requirements
- Prediction can be **slow.**

  Complexity of labeling 1 new data point: $O(pn + n \log k)$

  But kNN works best with lots of samples...

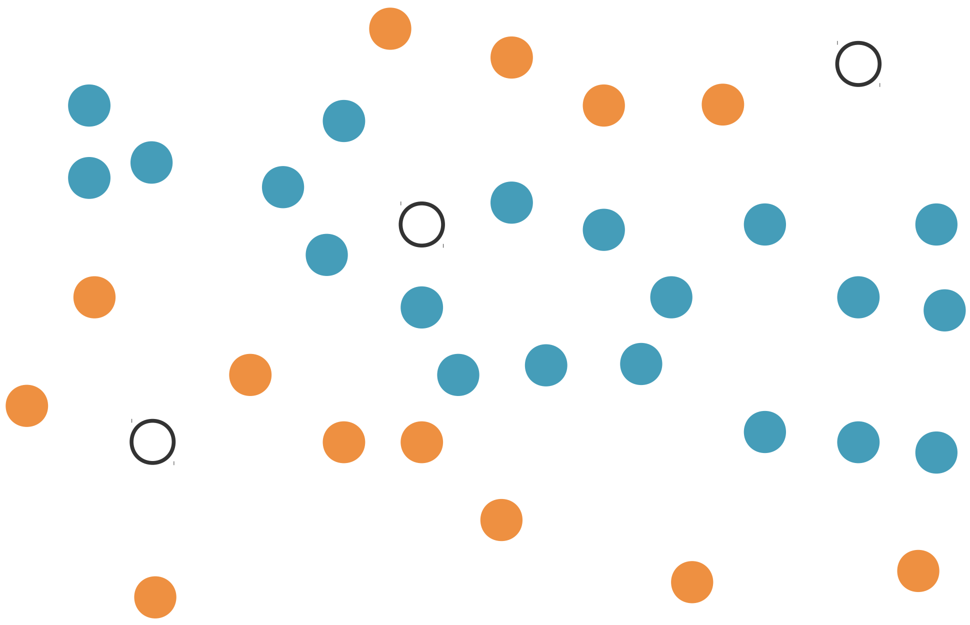
  → Efficient data structures (k-D trees)

  → Approximate solutions based on hashing
- kNN are fooled by **irrelevant attributes.**

  E.g. $p=1000$, only 10 features are relevant; distances become meaningless.

Decision boundary of kNN

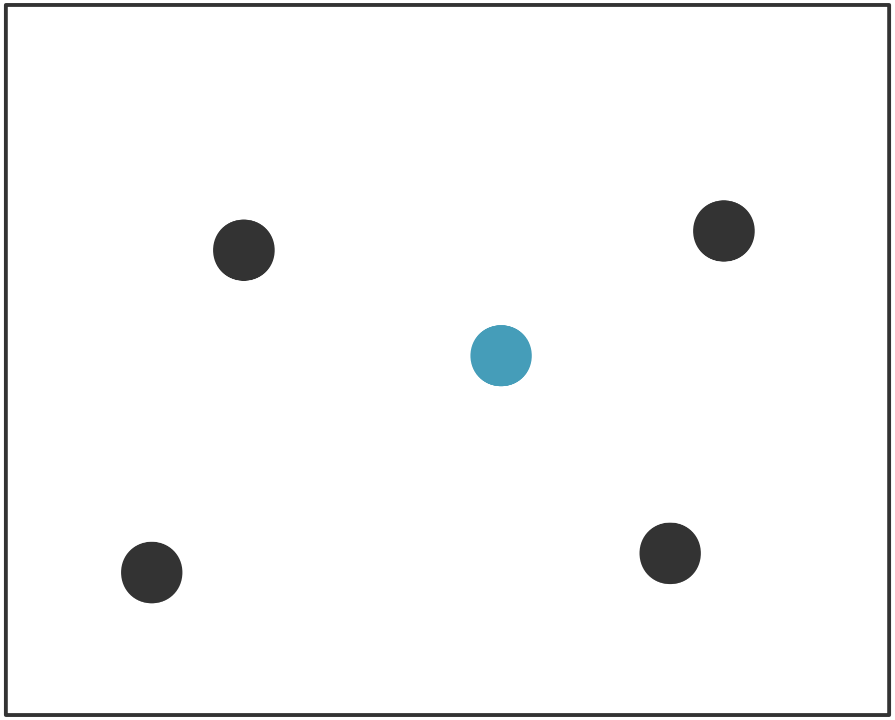
- Classification
- **Decision boundary:** Line separating the positive from negative regions.
- **What decision boundary is the kNN building?**



Voronoi tesselation

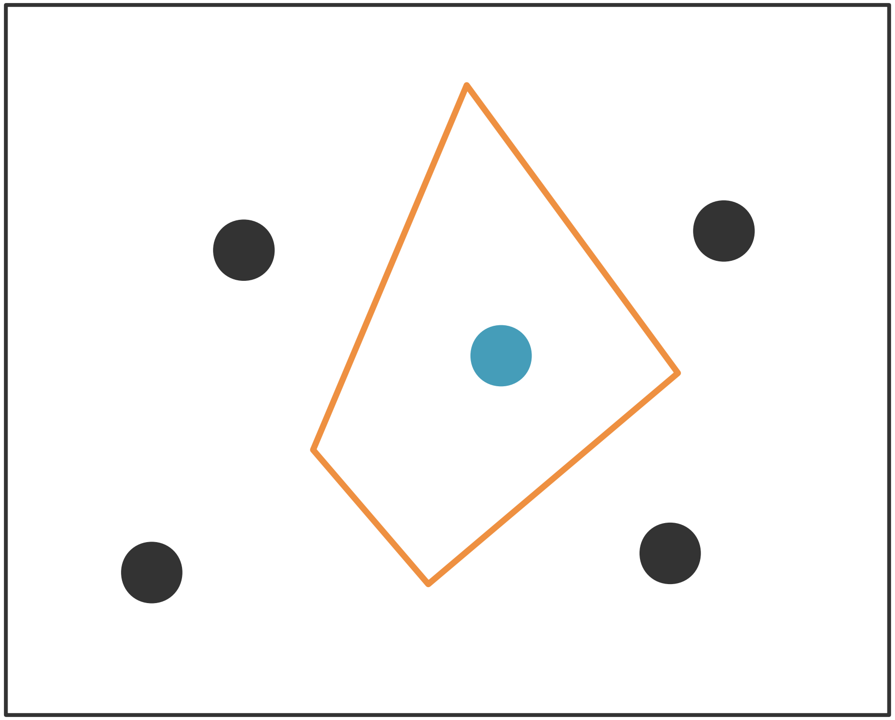
- **Voronoi cell** of **x**:
  - set of all points of the space closer to **x** than any other point of the training set
  - polyhedron
- **Voronoid tesselation** of the space: union of all Voronoi cells.

Draw the Voronoi cell of the blue dot.



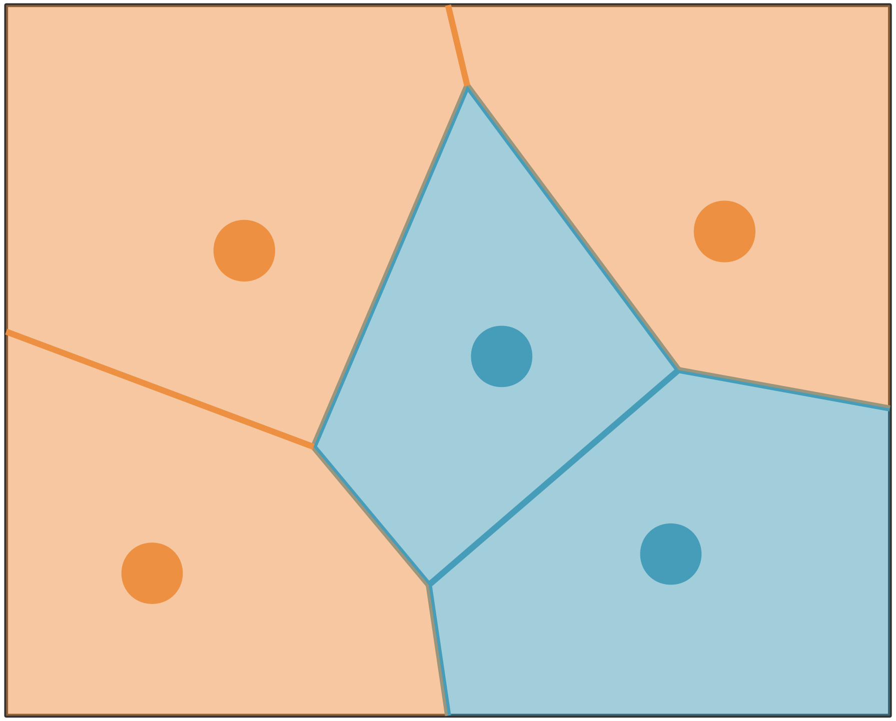
Voronoi tesselation

- **Voronoi cell** of **x**:
  - set of all points of the space closer to **x** than any other point of the training set
  - polyhedron
- **Voronoid tesselation** of the space: union of all Voronoi cells.



Voronoi tesselation

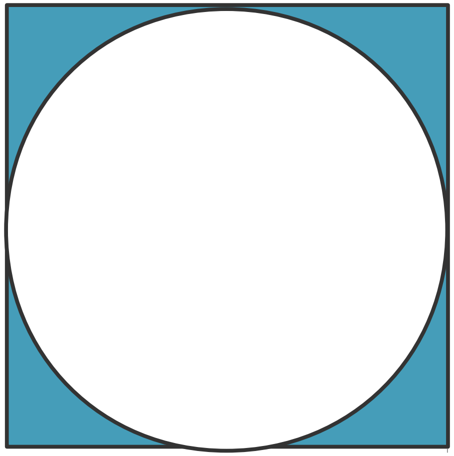
- The Voronoi tesselation defines the decision boundary of the 1-NN.



- The kNN also partitions the space (in a more complex way).

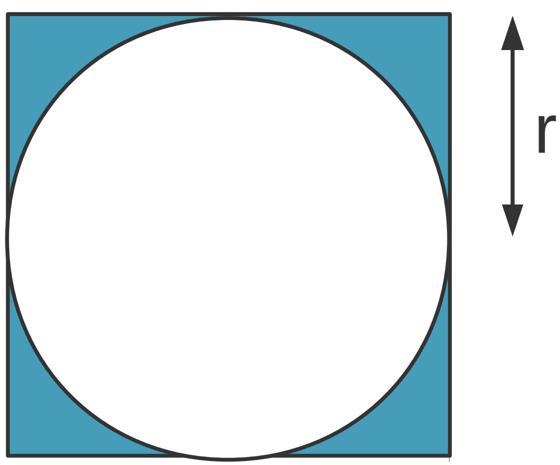
Curse of dimensionality

- Methods / intuitions that work in low dimension may not apply to high dimensions.
- **p=2: What fraction of the points within a square fall outside of the circle inscribed in it?**



Curse of dimensionality

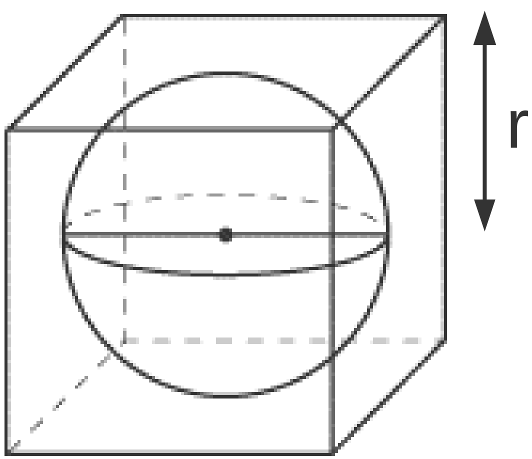
- Methods / intuitions that work in low dimension may not apply to high dimensions.
- **p=2: What fraction of the points within a square fall outside of the circle inscribed in it?**



$$1 - \frac{\pi r^2}{4r^2} = 1 - \frac{\pi}{4}$$

Curse of dimensionality

- Methods / intuitions that work in low dimension may not apply to high dimensions.
- **p=3: What fraction of the points within a cube fall outside of the sphere inscribed in it?**



$$1 - \frac{4/3\pi r^3}{8r^3} = 1 - \frac{\pi}{6}$$

Curse of dimensionality

- **Volume of a p-sphere:** $\frac{2r^p \pi^{p/2}}{p\Gamma(p/2)}$

The Gamma function Γ generalizes the factorial.
 Γ(n) = (n-1)!

- When p ↗ the proportion of a hypercube outside of its inscribed hypersphere approaches 1.

- What this means:
  - hyperspace is very big
  - **all points are far apart**
  - **dimensionality reduction needed (see Chap 11).**

kNN variants

- **ε-ball neighbors**
  - Instead of using the k nearest neighbors, use **all points within a distance ε** of the test point.
  - **What if there are no such points?**

kNN variants

- **Weighted kNN**
  - **Weigh the vote of each neighbor** according to the distance to the test point.

$$w_l = \exp\left(\frac{1}{2}d(\boldsymbol{x}, \boldsymbol{x}^l)\right)$$

  - Variant: **learn** the optimal weights [e.g. Swamidass, Azencott et al. 2009, Influence Relevance Voter]

Collaborative filtering

- **Collaborative filtering:** recommend items that similar users have liked in the past

    similar users = users with similar tastes

- **item-based kNN**
    - similarity between items: **adjusted cosine similarity**

Sum over the users that rated both item A and item B

$$s(A,B) = \frac{\sum_u (R(u,A) - \bar{R}(u))(R(u,B) - \bar{R}(u))}{\sqrt{\sum_u (R(u,A) - \bar{R}(u))^2 \sum_u (R(u,B) - \bar{R}(u))^2}}$$

Rating of item A by user u **Average rating by user u**

Collaborative filtering

- score of item A for user u:

$$S(u, A) = \frac{\sum_{B \in \mathcal{N}_u^k(A)} s(A, B) R(u, B)}{\sum_{B \in \mathcal{N}_u^k(A)} |s(A, B)|}$$

k nearest neighbors of A
according to s
among the items rated by user u

Summary

- **kNN**
  - very simple training
  - prediction can be expensive
- Relies on a “good” **distance/similarity** between instances
- **Decision boundary** = **Voronoi tesselation**
- **Curse of dimensionality:** the hyperspace is very big.