Department of COMPUTER SCIENCE

WARWICK
THE UNIVERSITY OF WARWICK

Machine Learning CS342

Lecture 4: Instance-based Learning: The k-NN algorithm

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Office hours (CS 307)

Mon 16:00-17:00 Fri 16:00-17:00

Last week summary:

Linear regression (OLS)
Ch1. R&G book

Machine Learning

Supervised Learning
- Regression ←
- Classification
- Ranking
- Structured Prediction

$\mathcal{D} = \{\mathbf{X}, \mathbf{t}\}, \quad e.g. \quad \mathbf{X} \in \Re^{N \times D}, \mathbf{t} \in \Re^{N}$

Unsupervised Learning
- Clustering
- Dimensionality Reduction
- Manifold Learning

$\mathcal{D} = \{\mathbf{X}\}, \quad \mathbf{X} \in \Re^{N \times D}$

Reinforcement Learning
- Markov Decision Process (e.g. Robotics)
- Multi-Agent Systems
- TD/Q-Learning (State-Action-Reward)

$\mathcal{D} = \{\mathbf{S}, \mathbf{A}, \mathbf{R}, \pi^*, \mathbf{V}\}$

Last week summary: Inputs X - Outputs t

$$\mathcal{D} = \{\mathbf{X}, \mathbf{t}\}$$

Further Training & Validation splits on this

Attributes, Dimensions, Features

D

Observations
Samples
Instances

N

Student reg. no.	ML grade	P. Skills grade	final degree
1	92%	84%	78%
2	54%	100%	62%
3	58%	50%	52%
4	85%	96%	72%
5	67%	98%	68%
6	75%	86%	72%
7	52%	100%	61%
8	82%	90%	85%

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \\ x_{41} & x_{42} \\ x_{51} & x_{52} \\ x_{61} & x_{62} \\ x_{71} & x_{72} \\ x_{81} & x_{82} \end{bmatrix} \qquad \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ t_4 \\ t_5 \\ t_6 \\ t_7 \\ t_8 \end{bmatrix}$$

$$\mathbf{X} \in \Re^{N \times D} \qquad \mathbf{t} \in \Re^{N}$$

Last week summary: Linear model

$$\hat{t}_n = \hat{w}_0 + \hat{w}_1 x_{n1} + \hat{w}_2 x_{n2} = \mathbf{x}_n \hat{\mathbf{w}} \qquad \hat{\mathbf{t}} = \mathbf{X}\hat{\mathbf{w}}$$

Squared Error Loss $\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2$

Find the parameters that minimise the Loss

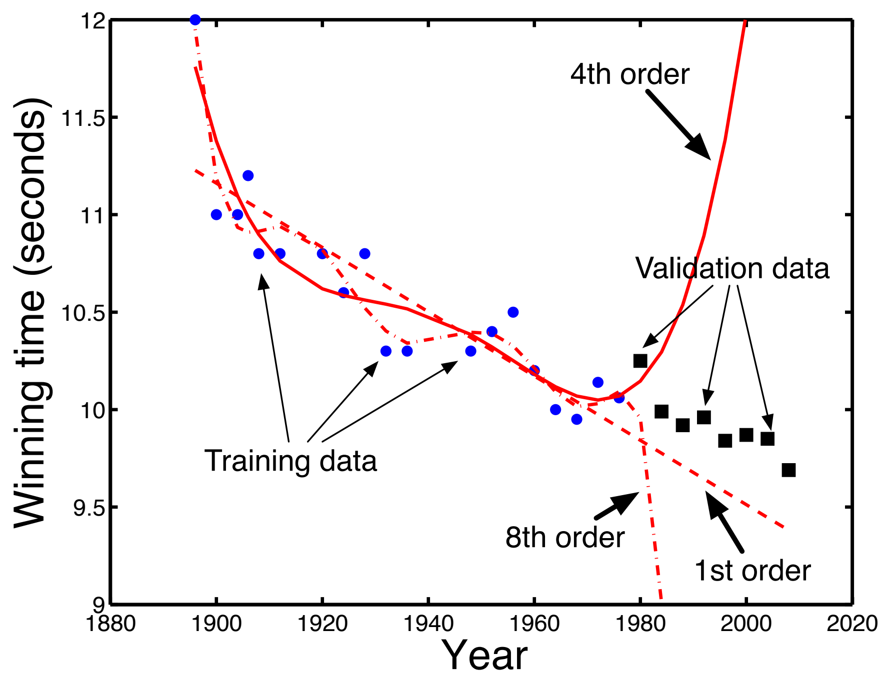
$$\widehat{w_0}, \widehat{w_1} \leftarrow \underset{w_0, w_1}{\operatorname{argmin}} \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}_n(t_n, f(x_n; w_0, w_1))$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} \to 0 \qquad \text{if} \quad \frac{\partial^2 \mathcal{L}}{\partial^2 \mathbf{w}} > 0 \quad \text{we are at a minima}$$

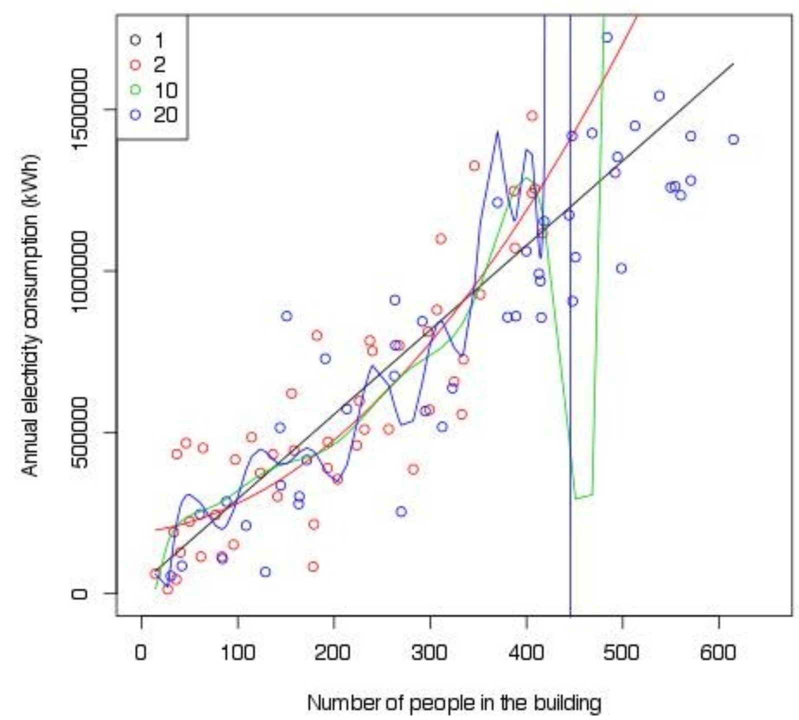
$$\widehat{\mathbf{w}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{t} \qquad \text{where} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1D} \\ 1 & x_{21} & \dots & x_{2D} \\ 1 & x_{N1} & \dots & x_{ND} \end{bmatrix}$$

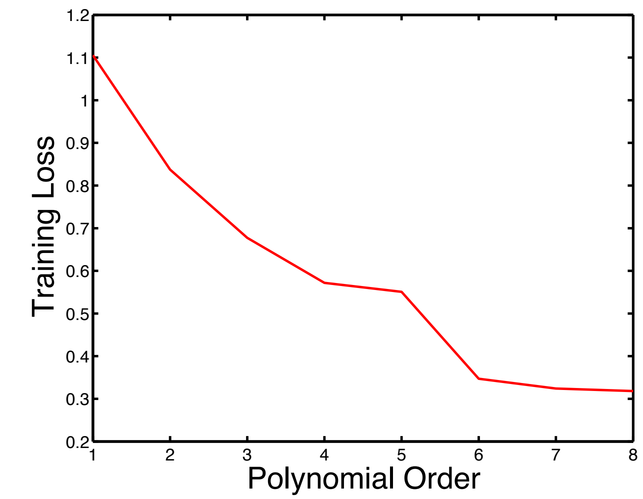
Last week summary: Overfitting & Cross-validation

Generalisation & Validation data

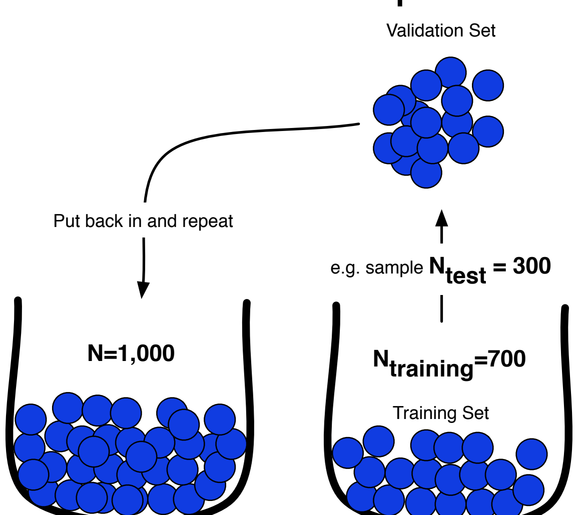


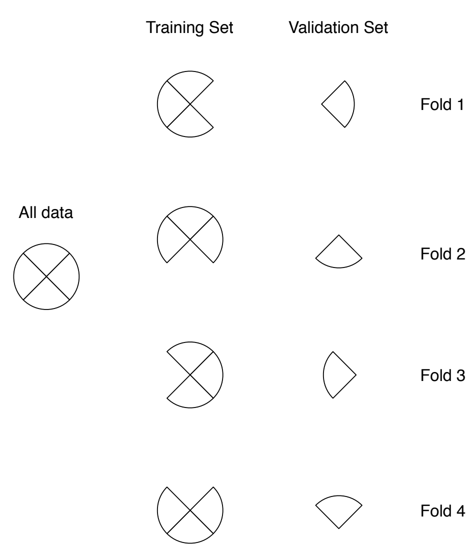
Overfitting and Curse of Dimensionality



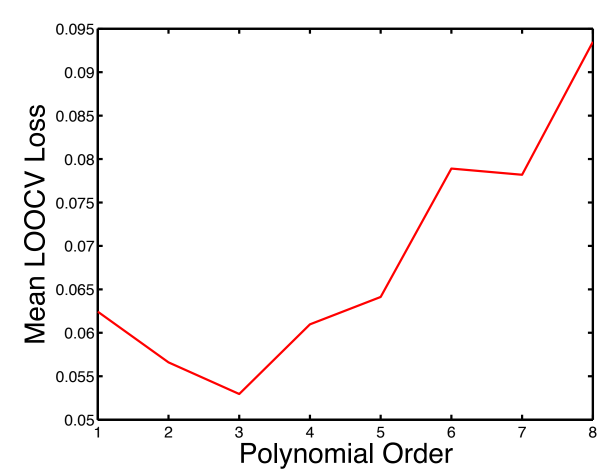


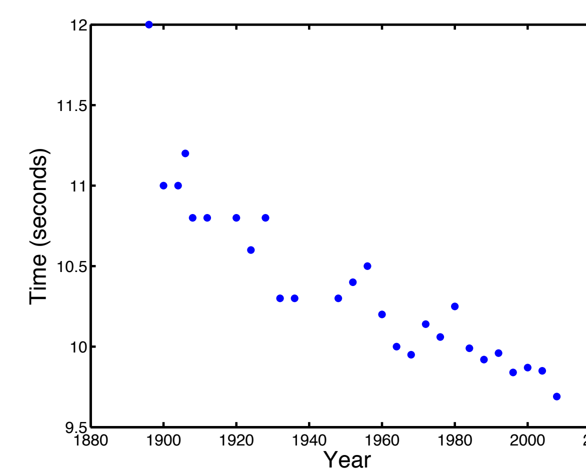
Bootstrap & Cross-validation





Model Selection and IID assumption





This week

Linear & Non-linear regression
Classification (k-NN, DTs)

Machine Learning

- **Supervised Learning**
  - Regression
  - Classification
  - Ranking
  - Structured Prediction

  $$\mathcal{D} = \{\mathbf{X}, \mathbf{t}\}, \quad e.g. \quad \mathbf{X} \in \Re^{N \times D}, \mathbf{t} \in \Re^{N}$$

- **Unsupervised Learning**
  - Clustering
  - Dimensionality Reduction
  - Manifold Learning

  $$\mathcal{D} = \{\mathbf{X}\}, \quad \mathbf{X} \in \Re^{N \times D}$$

- **Reinforcement Learning**
  - Markov Decision Process (e.g. Robotics)
  - Multi-Agent Systems
  - TD/Q-Learning (State-Action-Reward)

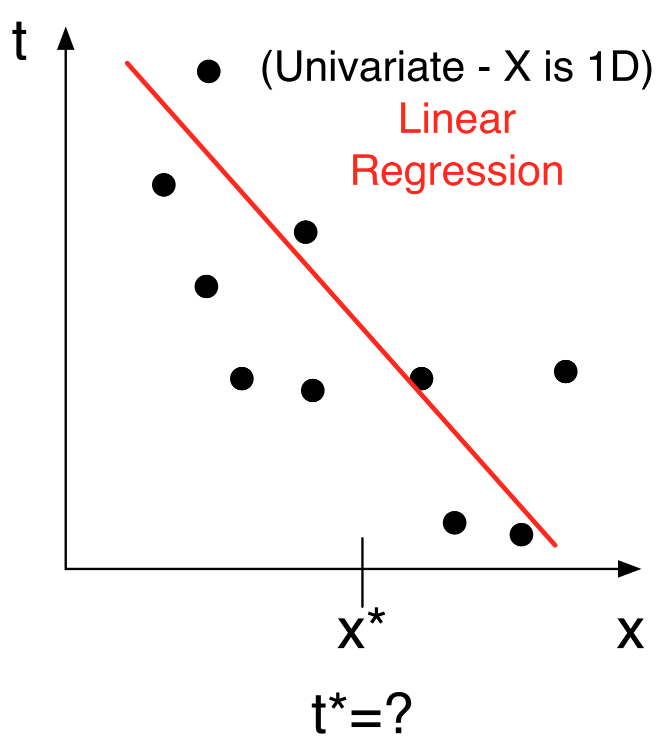
  $$\mathcal{D} = \{\mathbf{S}, \mathbf{A}, \mathbf{R}, \pi^*, \mathbf{V}\}$$

Instance-based Learning (Regression & Classification)

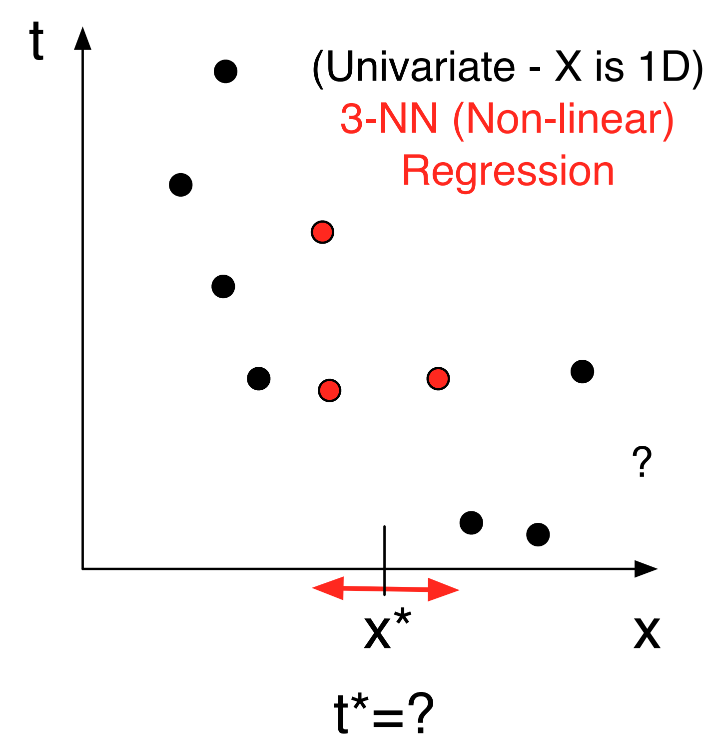
T. Mitchell book, Ch.8

Instance-based learners are all the machine learning algorithms that ***do not*** *construct an explicit description of the target function (like OLS) but store the training examples (instances) and use them,* ***and a notion of distance from them****, to generalise to unseen data.*

Regression: t is continuous



Training: Learn the best line/plane
Predict: Use the line/plane

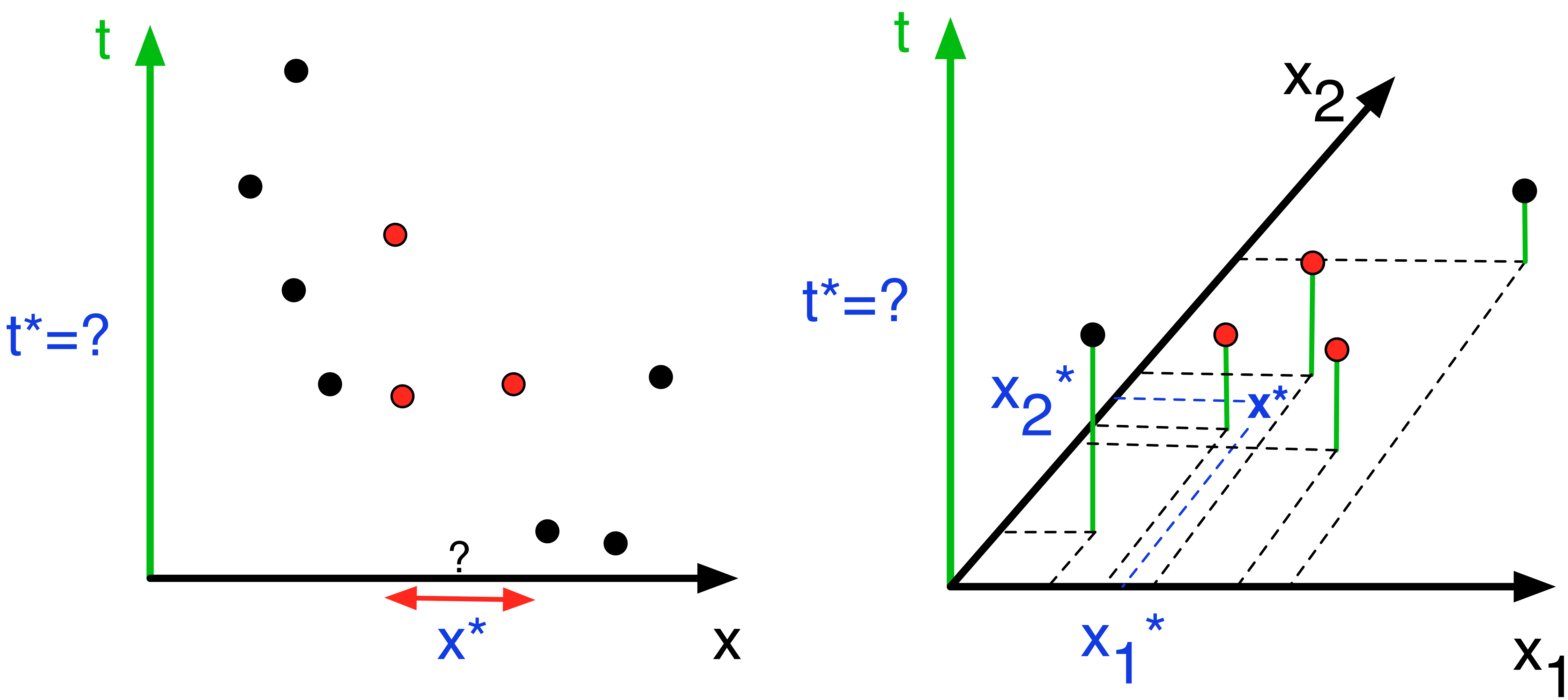


Training: Store the training data
Predict: Use the "closest" observations

What if we have 2 or more attributes (dimensions) for X?

Univariate (x is 1D)

Multivariate (x is 2D)



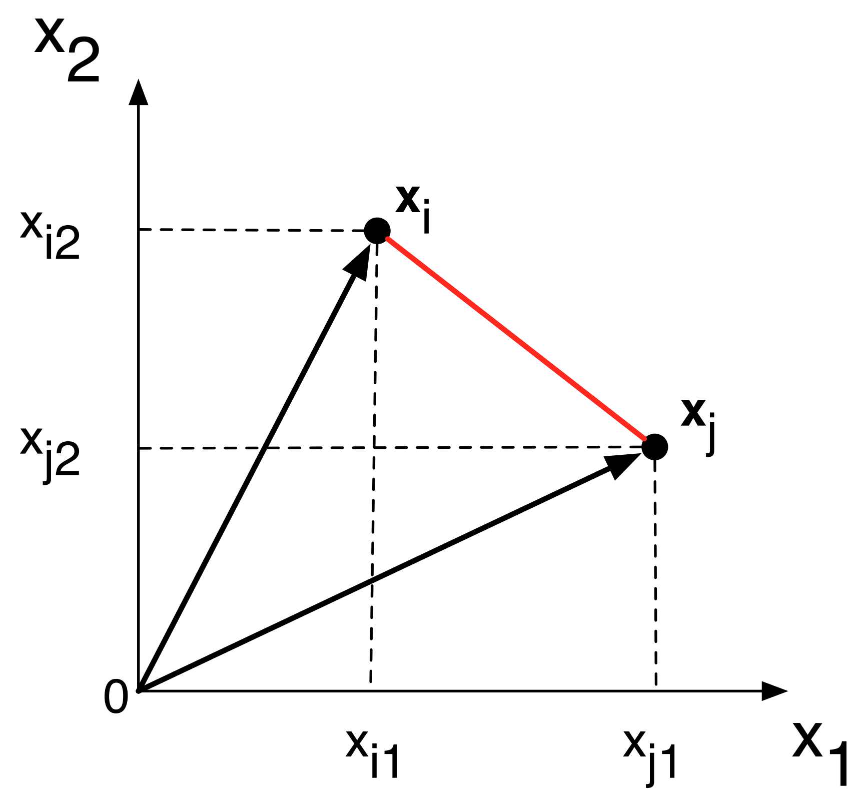
Need a distance metric

Euclidean Distance

Euclidean (L2) Distance
between x_i and x_j?

Input space
Univariate (x is 1-D scalar)

Input space
Multivariate (**x** is 2-D vector)



$$\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{iD}] \quad \in \quad \Re^D$$

$$\mathbf{x}_j = [x_{j1}, x_{j2}, \ldots, x_{jD}] \quad \in \quad \Re^D$$

For any D $\qquad d^{\text{Euclidean}}(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{d=1}^{D} (x_{id} - x_{jd})^2}$ $\qquad$ Remember Lp norm?

Other distances? Lp norms and Distances

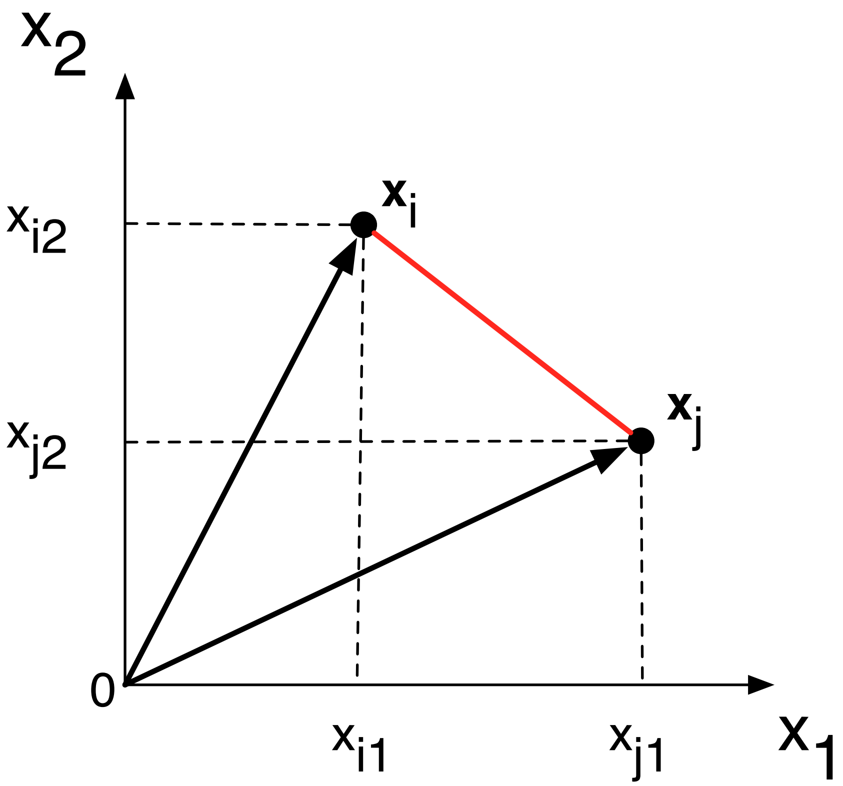
for a D-dimensional vector $\mathbf{x}_n$ the Lp norm is:

$$\mathrm{L}_p = \left(\sum_{d=1}^{D} |x_{nd}|^p \right)^{\frac{1}{p}}$$

Every norm (e.g. L1 for p=1, L2 for p=2) induces a *metric distance*

for p=2, Euclidean (L2) norm:

$$\mathrm{L}_2 = \left(\sum_{d=1}^{D} |x_{nd}|^2 \right)^{\frac{1}{2}} = \sqrt{\sum_{d=1}^{D} |x_{nd}|^2}$$



So L2 distance between $\mathbf{x}_i$ and $\mathbf{x}_j$:

$$\mathrm{L}_2(\mathbf{x}_i, \mathbf{x}_j) \overset{\text{Euclidean}}{=} d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{d=1}^{D} (x_{id} - x_{jd})^2}$$

Manhattan distance (L1)

Can you use the Lp norm definition to write the L1 (p=1) distance between **x**$_i$ and **x**$_j$?

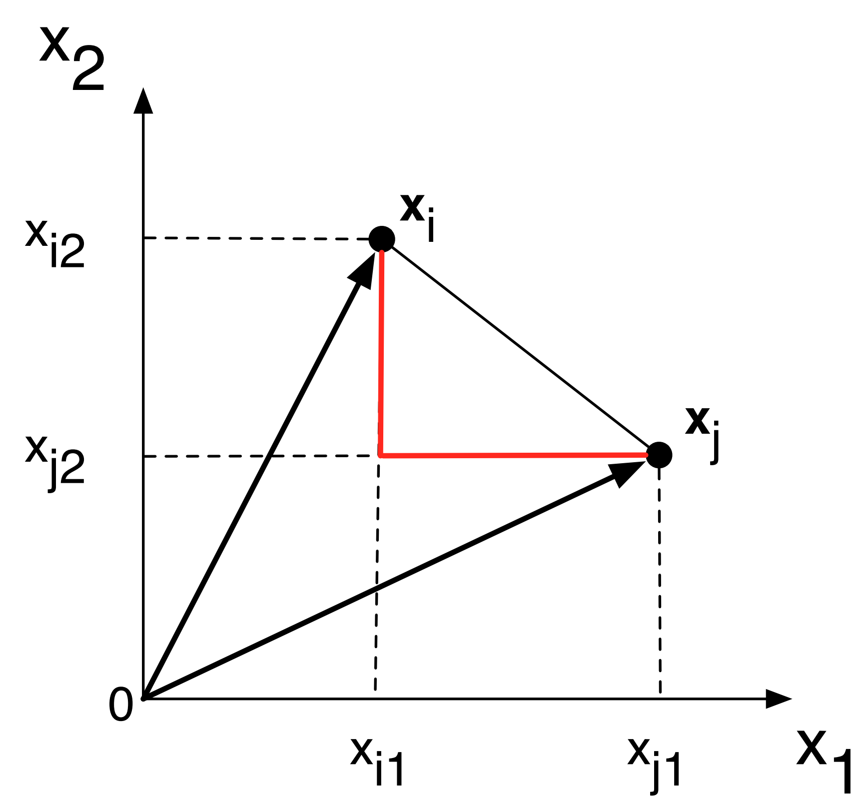
$$\mathrm{L}_p = \left(\sum_{d=1}^{D} |x_{nd}|^p \right)^{\frac{1}{p}}$$

$$d^{\text{Manhattan}}(\mathbf{x}_i, \mathbf{x}_j) = \sum_{d=1}^{D} |x_{id} - x_{jd}|$$

Manhattan (L1) Distance between x_i and x_j?

Input space
Univariate (x is 1-D scalar)

Input space
Multivariate (**x** is 2-D vector)



Distance for categorical data?

$\mathbf{x}_i$	1	0	1	1
$\mathbf{x}_j$	0	1	1	1

Hamming distance

$$d(\mathbf{x}_i, \mathbf{x}_j) = \sum_{d=1}^{D} \begin{cases} 1 & \text{if} \quad x_{id} \neq x_{jd} \\ 0 & \text{if} \quad x_{id} = x_{jd} \end{cases}$$

basic k-NN algorithm for regression

a.k.a. Lazy learning: No real training step..

Training:

- For each training example (input-output pair $\mathbf{x}_n, t_n$), add the example to the list *training_examples*

Regression:

- Choose k, the number of neighbours we want
- Choose the distance function (e.g. Euclidean distance)
- Given a query instance **x*** to predict its output t*
  - Find $\mathbf{x}_1 \ldots \mathbf{x}_k$ the k instances that are **nearest** to **x*** using the selected distance
  - Return prediction: $t^* \leftarrow \frac{\sum_{i=1}^{k} t_i}{k}$

Notes:

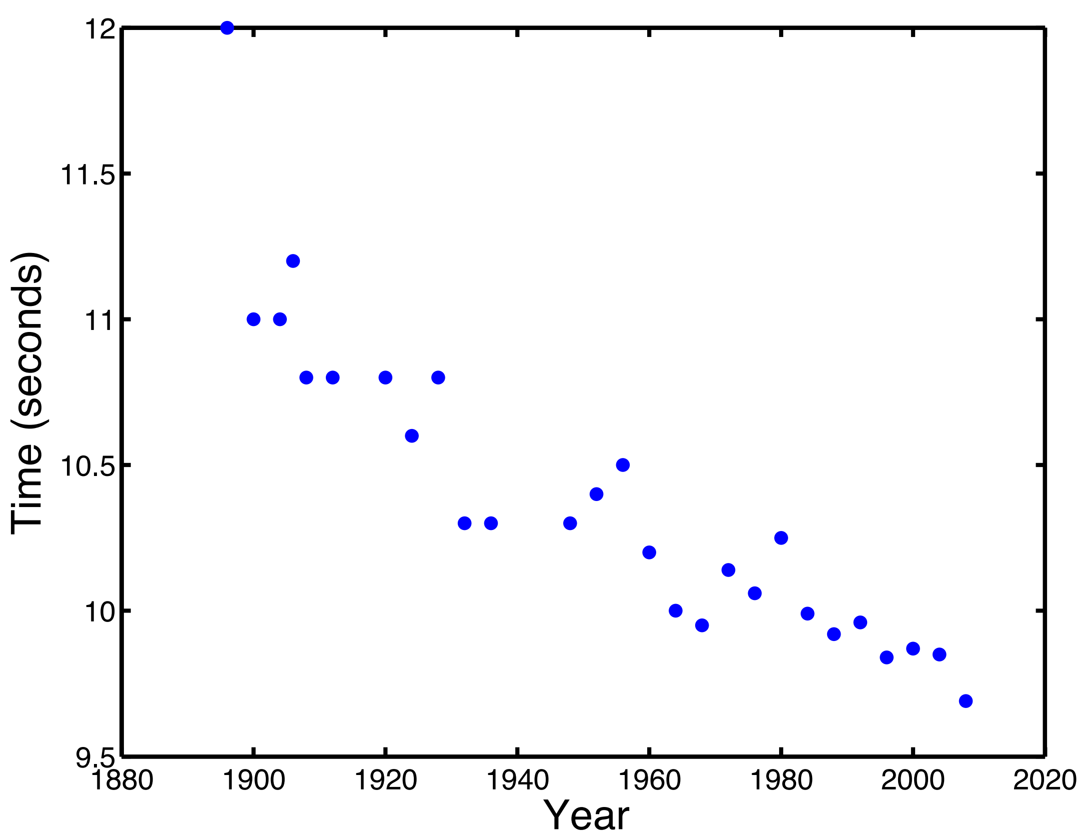
- i iterates over k neighbours
- t* is for single test point

Regression vs Classification

Regression: targets **t** are continuous values

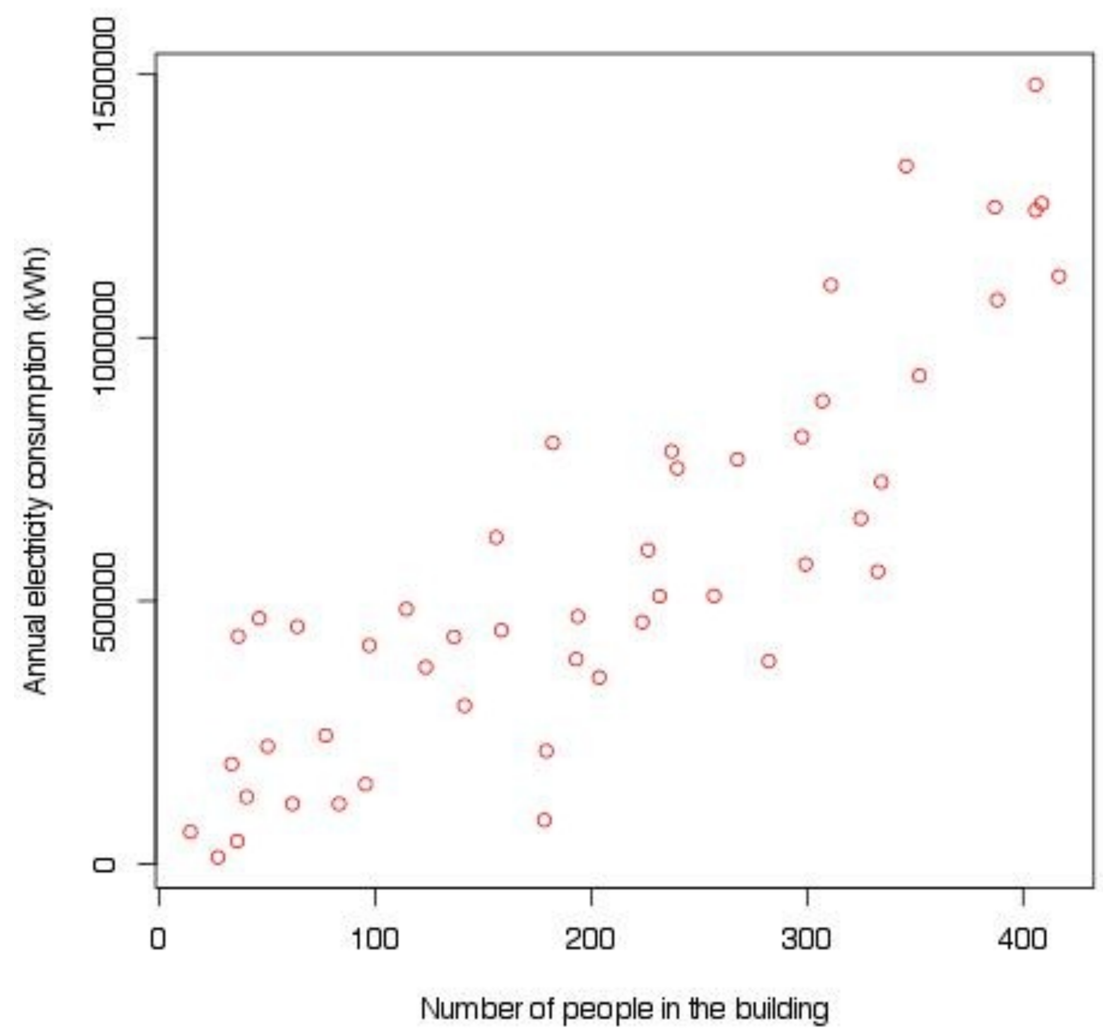
We can visualise the target as an additional dimension

t



x

t



In both cases we have one attribute so x is 1D

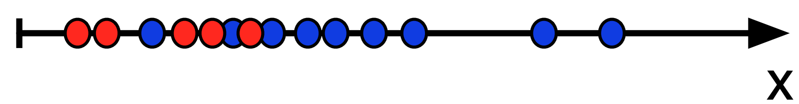
x

Regression vs Classification

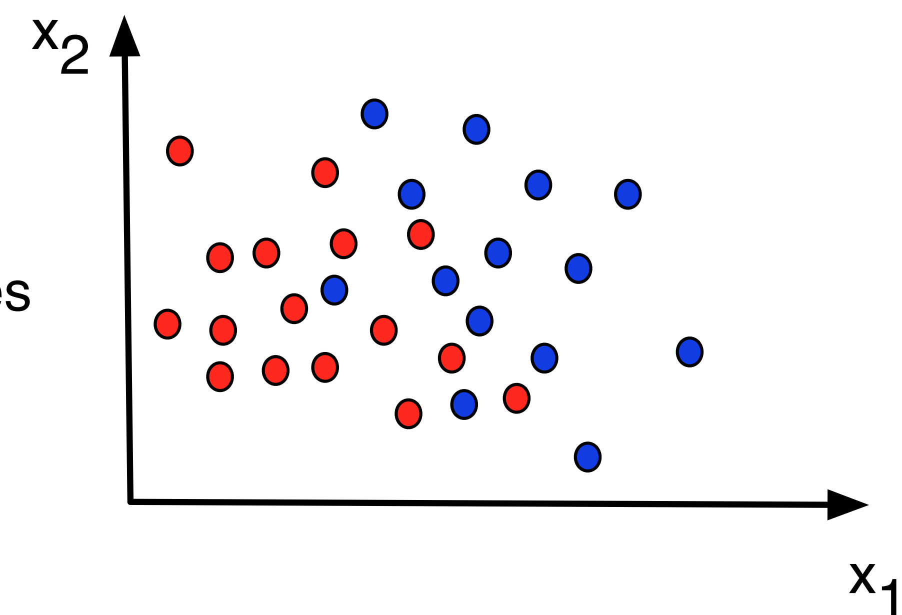
Classification: targets **t** are discrete values

We can visualise the target as different colour for each class

Inputs have one attribute
so 1D input space



Inputs have two attributes
so 2D input space



Binary Classification

$$t_n \in \{-1, 1\}$$

Multiclass/Multinomial Classification

$$t_n \in \{1, 2, \ldots, C\}$$

k-NN for classification?

Classification

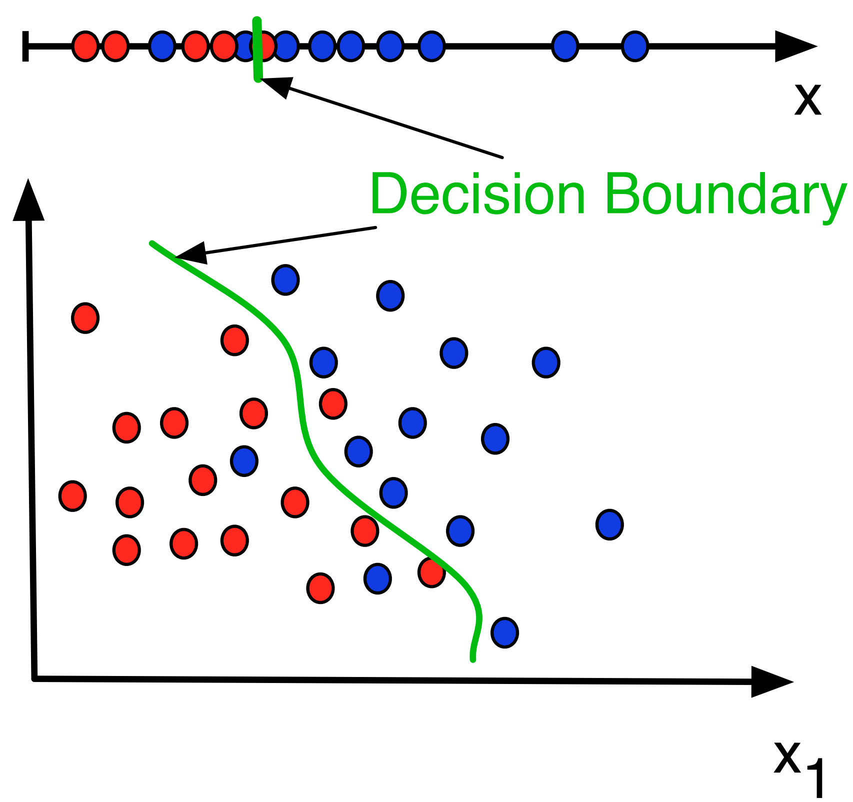
- The goal is to assign instances/inputs to target classes

$$t_n \in \{-1, 1\} \qquad\qquad t_n \in \{1, 2, \ldots, C\}$$

- The boundary between the classes where it is ***equiprobable to belong to either class*** is called the **decision boundary**

Inputs have one attribute so 1D input space

Inputs have two attributes so 2D input space



Classification with k-NN

Training:

- For each training example (input-output pair $\mathbf{x}_n, t_n$), add the example to the list *training_examples*

(Binary) Classification:

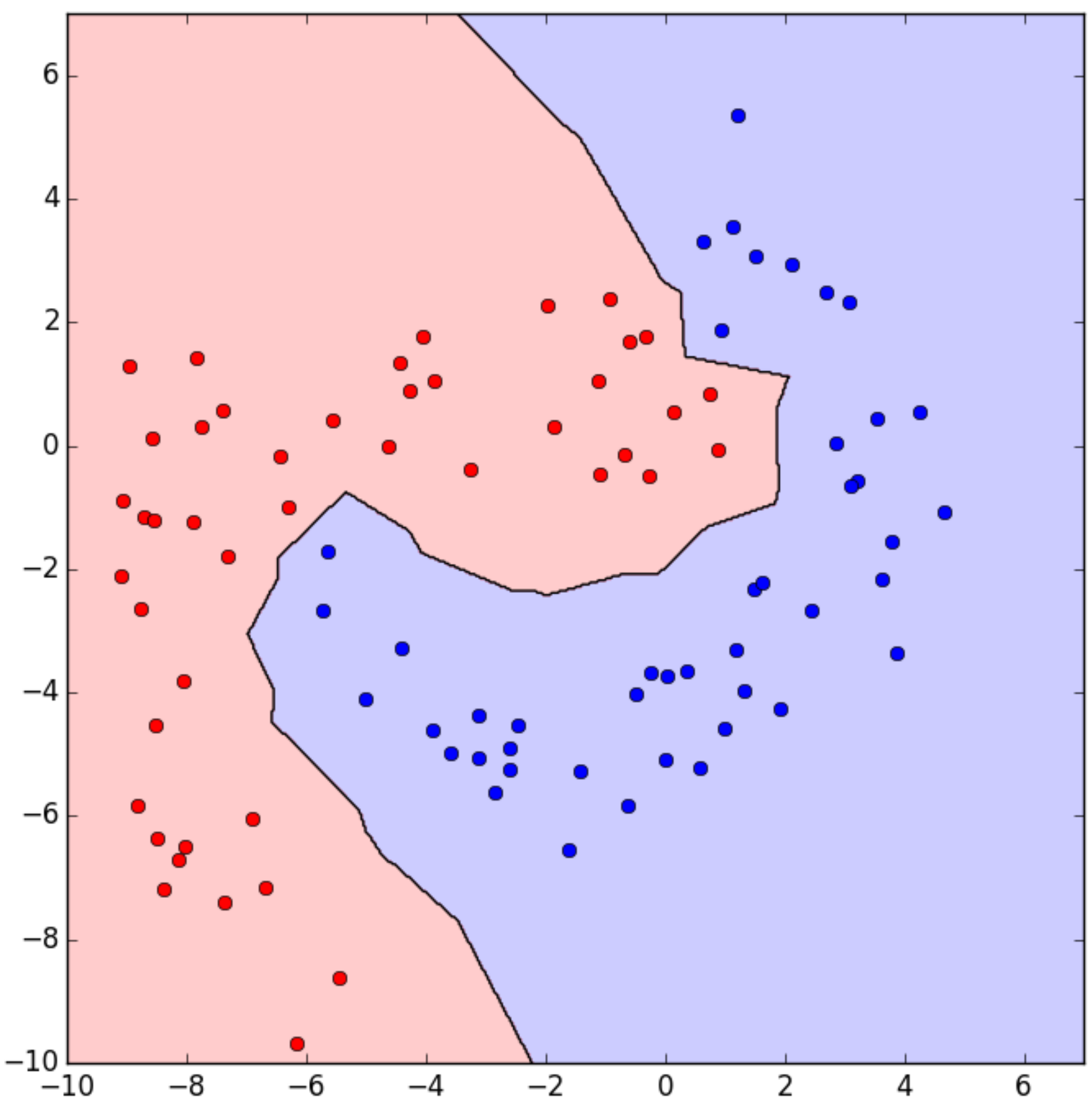
- Choose k, the number of neighbours we want
- Choose the distance function (e.g. Euclidean distance)
- Given a query instance **x*** to predict its output t*
  - Find $\mathbf{x}_1 \ldots \mathbf{x}_k$ the k instances that are **nearest** to **x*** using the selected distance
  - Return prediction: $t_n^* \leftarrow \text{majority}(t_1, \ldots, t_k)$

or more formally:

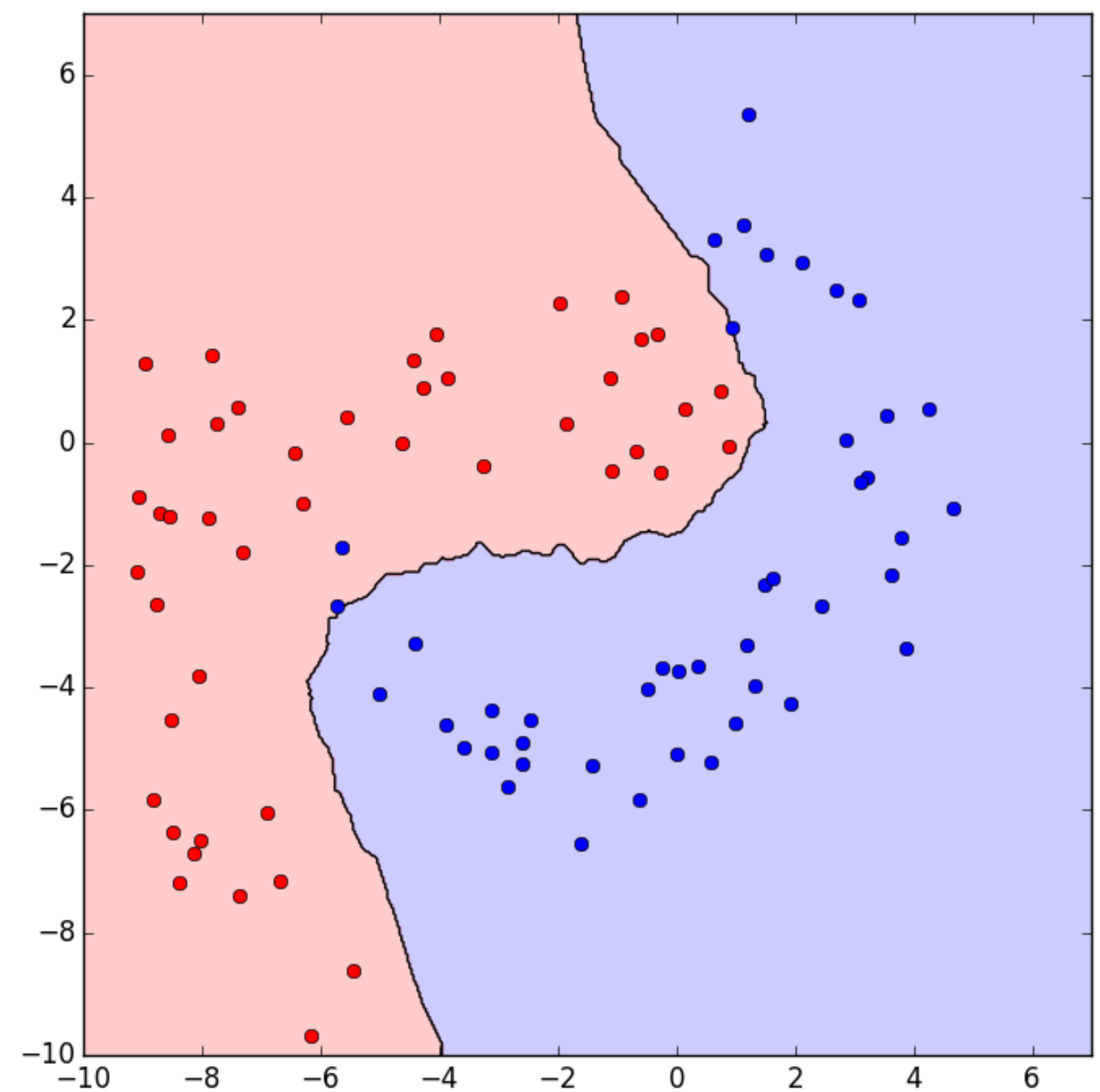
$$t_n^* \leftarrow \underset{u \in \{-1,1\}}{\text{argmax}} \sum_{i=1}^{k} \delta(u, t_i) \qquad \text{where } \delta(a,b) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise} \end{cases}$$

k-NN Classification

k=1



k=13

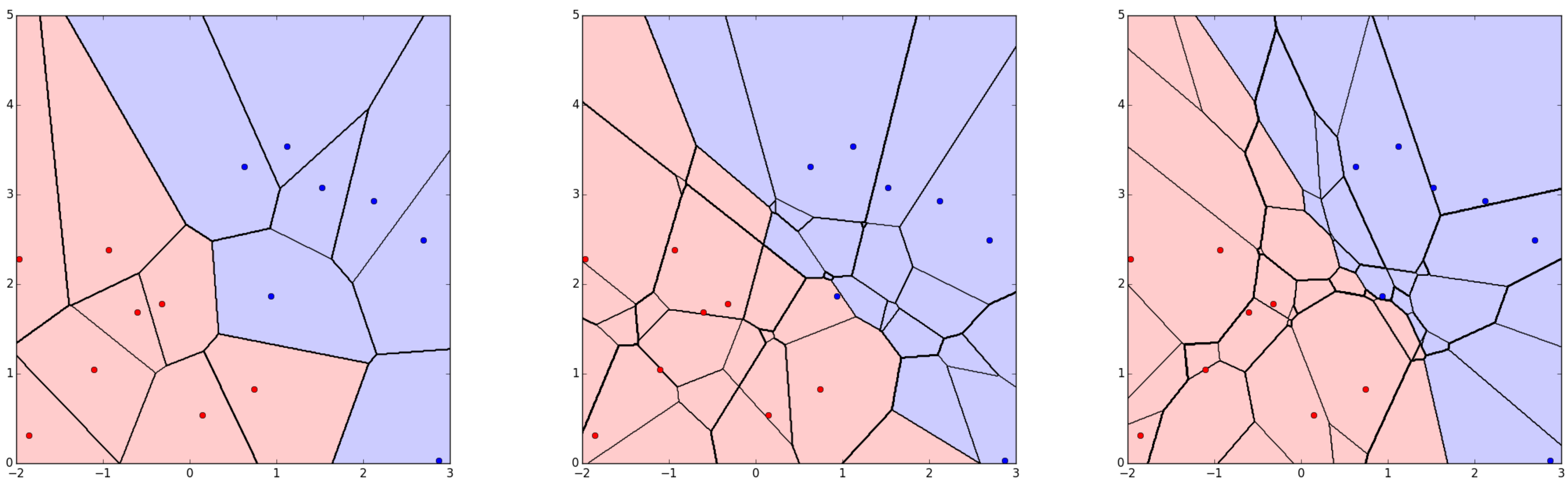


Piece-wise linear decision boundary

k-NN Classification: Effect of k

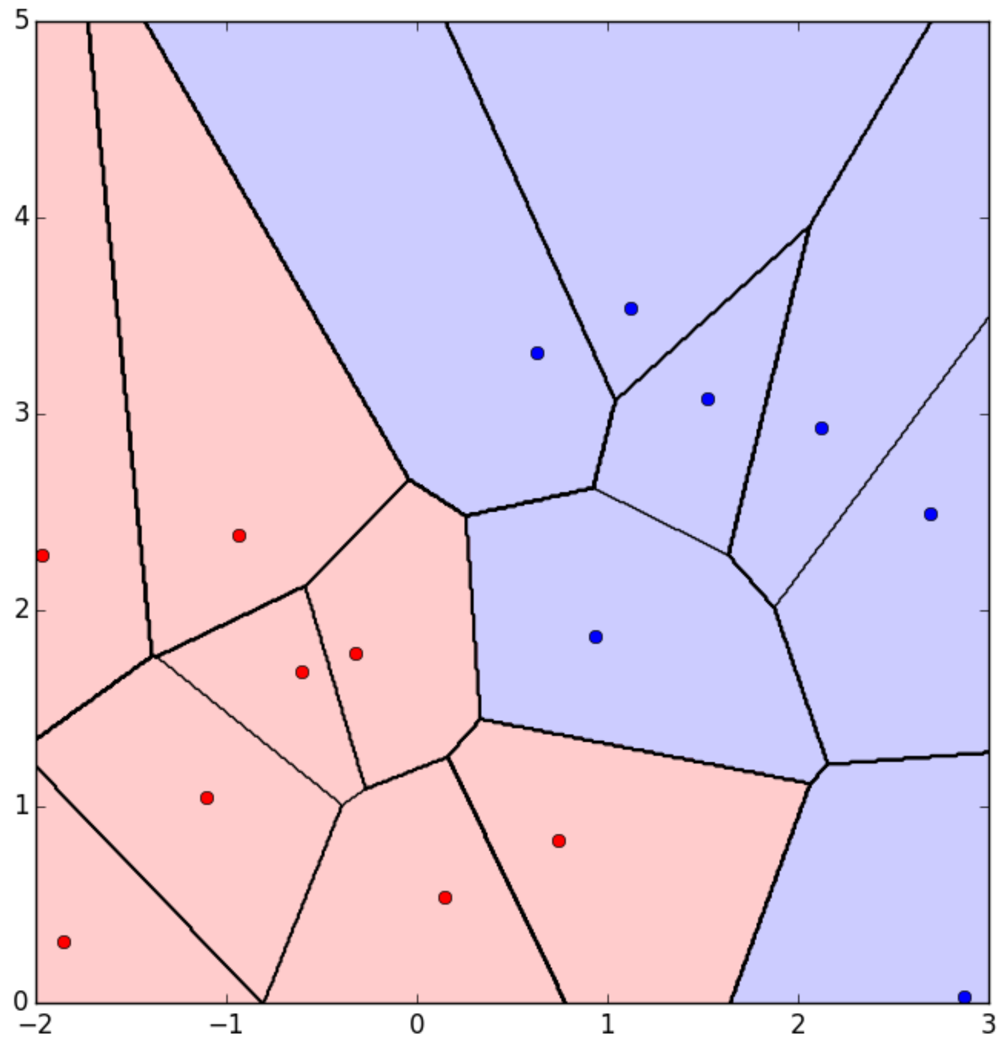
- k controls the complexity of the hypothesis we learn
- If k even then we need to resolve ties (in classification)
- As k increases we utilise more neighbours
- More neighbours = smoother decision boundary = less complex boundary
- k-NN creates Voronoy tessellations

k=1 k=3 k=5

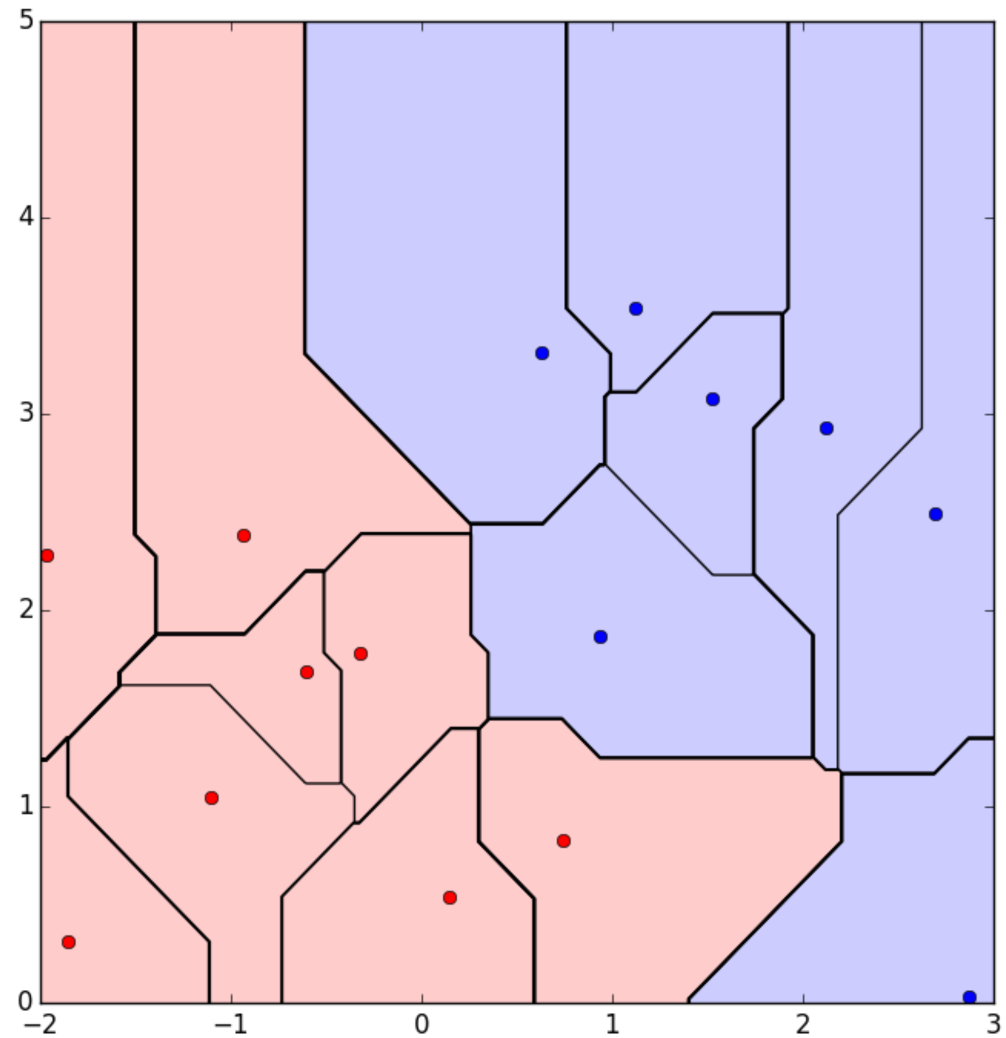


k-NN Classification: Effect of distance metric (L1 vs L2)

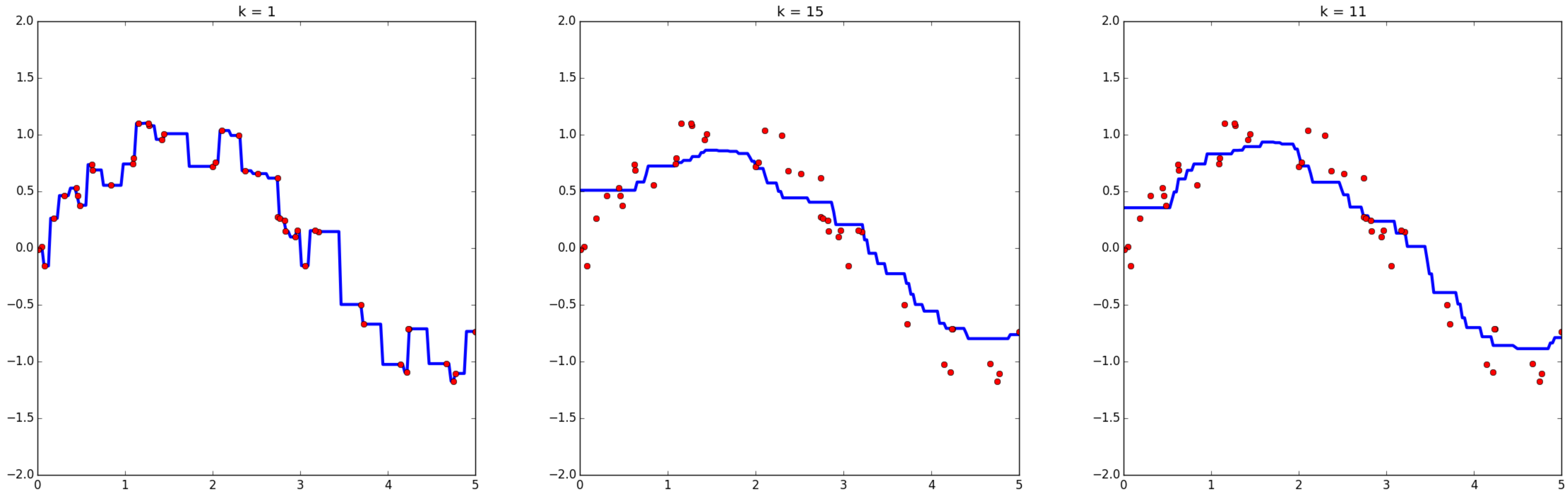
k=1, L2 (Euclidean) distance



k=1, L1 (Manhattan) distance



k-NN Regression: Effect of k



As we increase k, smoother piece-wise linear function

Boundary effects

Distance-weighted k-NN

- Weigh the vote of each neighbour by its distance to the observation
- Can help break ties when k is even
- Can help deal with noisy data and outliers

Regression:

$$t^* \leftarrow \frac{\sum_{i=1}^{k} w_i t_i}{\sum_{i=1}^{k} w_i}$$

$$w_i = \frac{1}{d(\mathbf{x}_i, \mathbf{x}^*)^2}$$

Classification:

$$t_n^* \leftarrow \underset{u \in \{-1,1\}}{\operatorname{argmax}} \sum_{i=1}^{k} w_i \delta(u, t_i)$$

$$\text{where } \delta(a,b) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise} \end{cases}$$

Remarks on k-NN

- Vanilla k-NN will not perform well in high-D as distances “break” in high-D
- In high-D, data concentrates so distances go to extremes
- Learn which attributes are important and weight these dimensions more
- Assign weights for every dimension and learn via e.g. cross-validation
- Can use tree data structures to improve search time for neighbours
- High computational cost to store all the training data in big data settings

Very simple algorithm but very successful over the years