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University of Applied Sciences
Western Switzerland

MSE | MASTER OF SCIENCE IN ENGINEERING

Machine Learning

F-MachLe

2. K-NN - an intuitive classification and regression system Curse of dimensionality

Jean Hennebert
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Plan - Supervised Learning for Classification tasks

2.1 Recap and examples

2.2 Intuitive classification with K-NN

2.3 Use case - K-NN for an image classification task

2.4 Regressor K-NN

2.4 The curse of dimensionality

Practical Work 2

2.1 Recap and examples

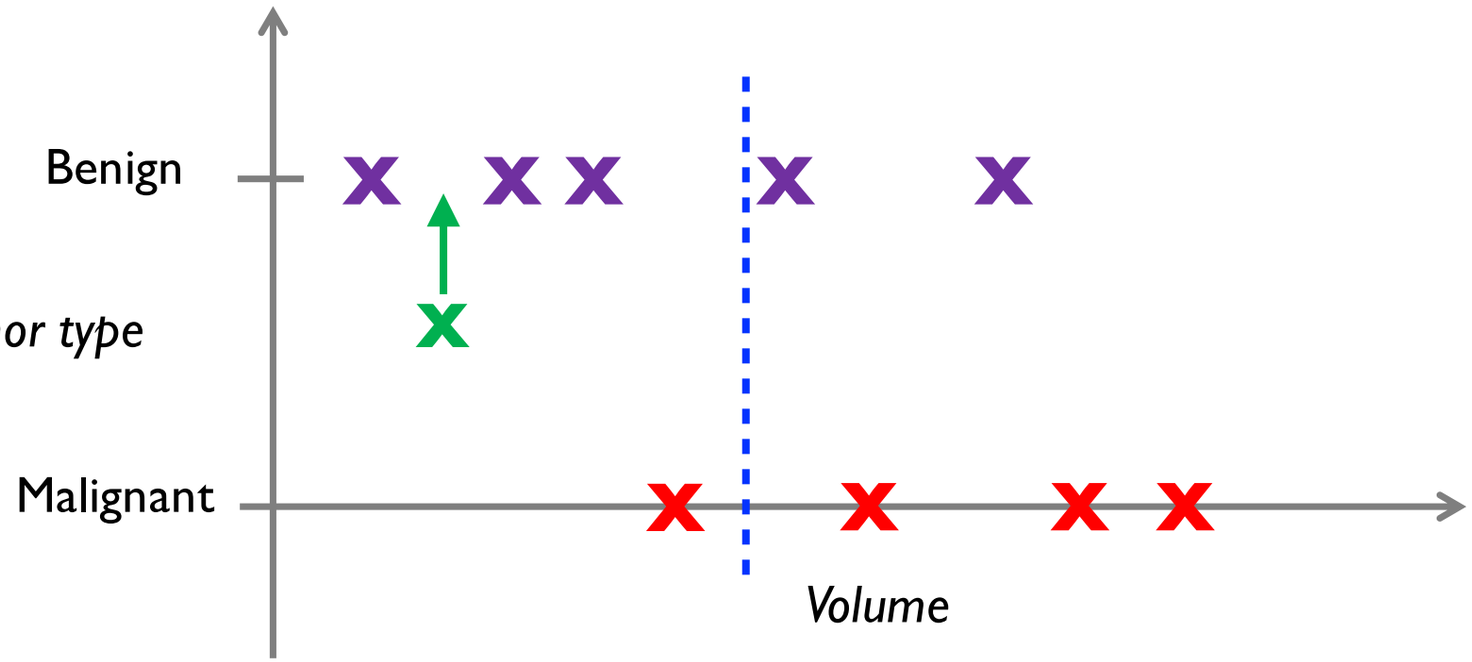
Classification task

Supervised learning - classification tasks

A **classification task** maps inputs **x** to a finite set of discrete outputs **y**. The outputs are the class labels corresponding to the different categories we want to predict.

- Usually classes are **mutually exclusive**, i.e. only one label is output of the system.
  - However, some systems are said **multi-label** when a given input x belongs to more than one class.
- 2-class systems are sometimes called **detection** or **verification** systems, where the objective is to answer yes/no questions
  - Biometric example: *Is this the face of Sheldon?* *Is the identity verified?*
  - Warship example: *Is a torpedo going to hit us?* *Is a torpedo detected?*

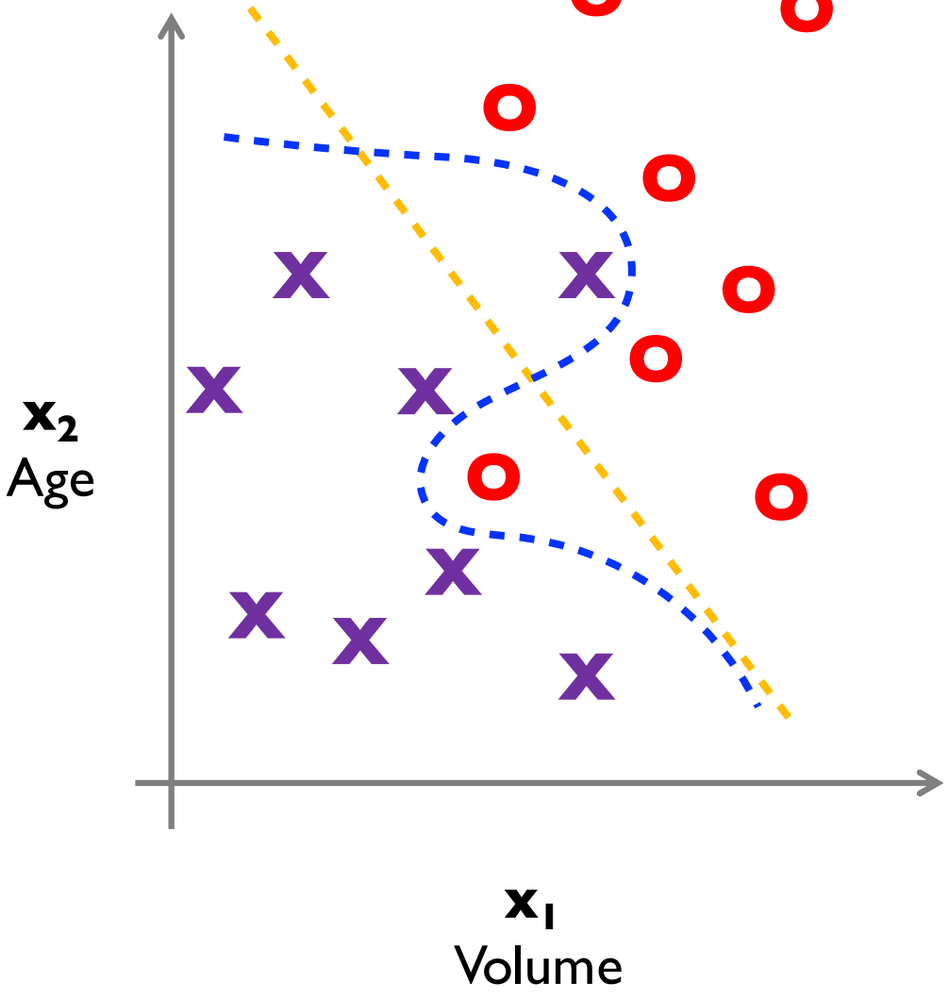
Supervised learning example 2 - tumour classification



The output of the system is discrete: this is called a **classification**

- We want to **categorise** a tumour into two classes: B or M
- We have a set of examples with the *right answers*
- We build a mathematical model explaining the mapping: *class = h(volume)*
  - In this case a simple threshold
- We can use the model to **classify** a new tumour

Supervised learning example 2 - tumour classification



- A typical way to increase the performance is to take into account more **features**
  - the input is becoming a vector with 2 components in this example
- The mapping function is *class = h(x1,x2)*
  - in yellow a linear model
  - in blue a non-linear model
- What other features could we bring in?
  - smoking quantity, family history, …

Tip: adding relevant features may increase performance. However this usually requires to have more data. See curse of dimensionality https://en.wikipedia.org/wiki/Curse_of_dimensionality

Some notations

$\mathbf{x}$	input variable of the system, also called **input feature**
y	output variable of the system, also called **target output**
$\widehat{y}$	**gotten output**, as computed by the mapping function
$(\mathbf{x}, y)$	a **training sample** (pair of feature and corresponding target)
$(\mathbf{x}_n, y_n)$	the training sample at index n in the training set ("in row" n)
N	the total number of training samples in the training set

The **training set** can then be noted

$$\{(\mathbf{x}_n, y_n); n = 1, \ldots, N\}$$

D	the dimension of the input space (x is a vector if $D > 1$)
$x_{n,d}$	the d'th coefficient of n'th training vector $\mathbf{x}_n$ (scalar value)

We can also define the **design matrix** X as the N-by-D matrix that contains the training examples' input values in its rows :

2.2 Intuitive classification with k-nn

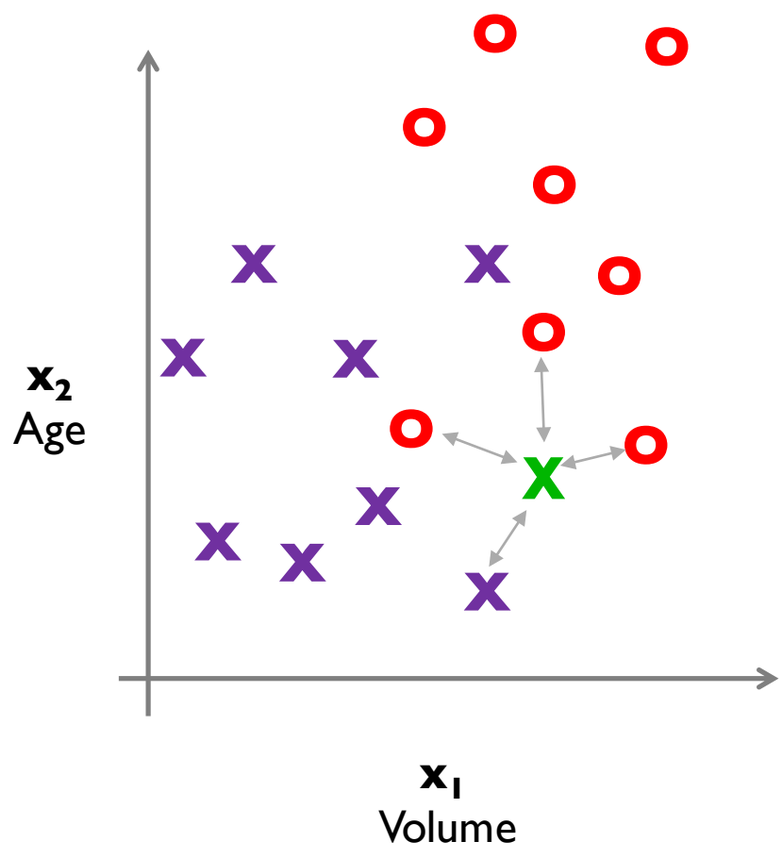
By Balu Ertl https://upload.wikimedia.org/wikipedia/commons/5/54/Euclidean_Voronoi_diagram.svg

k-nearest neighbour algorithm

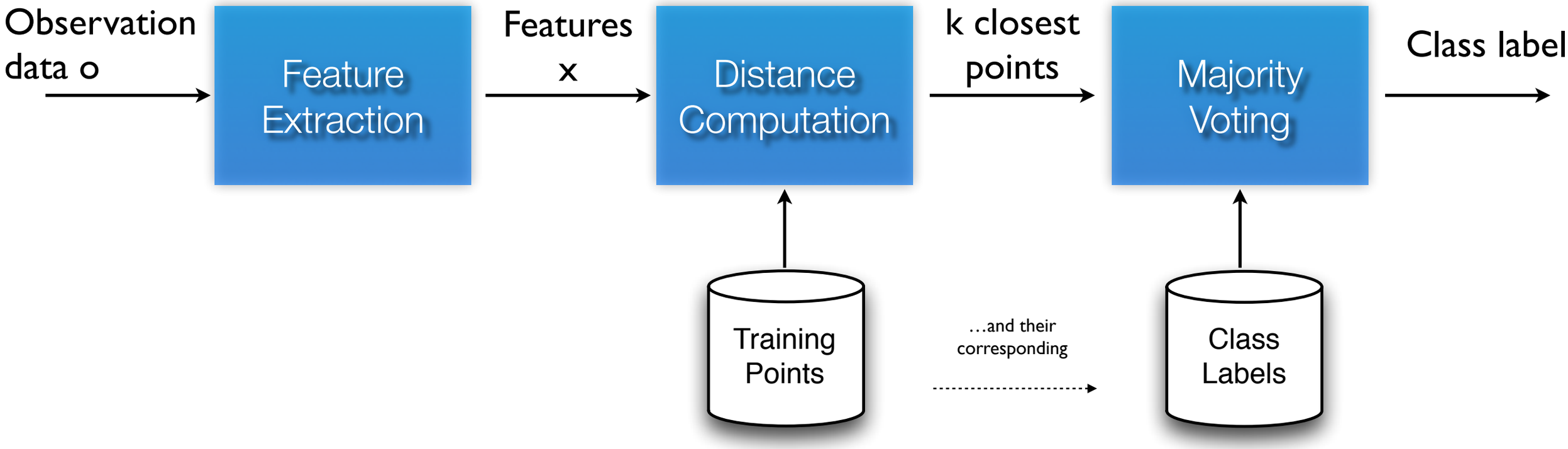
The **k-nearest neighbour** or **k-nn** algorithm is a method that classifies unlabelled examples based on their *similarity* with examples in the training set.

- The method requires
  - a parameter value *k*, the number of neighbour we consider to take the decision
  - a set of labeled examples
  - a distance metric
  - a voting strategy

With k=4 in this example, the new sample X is labelled O.



Intuitive classification: the k-nn approach



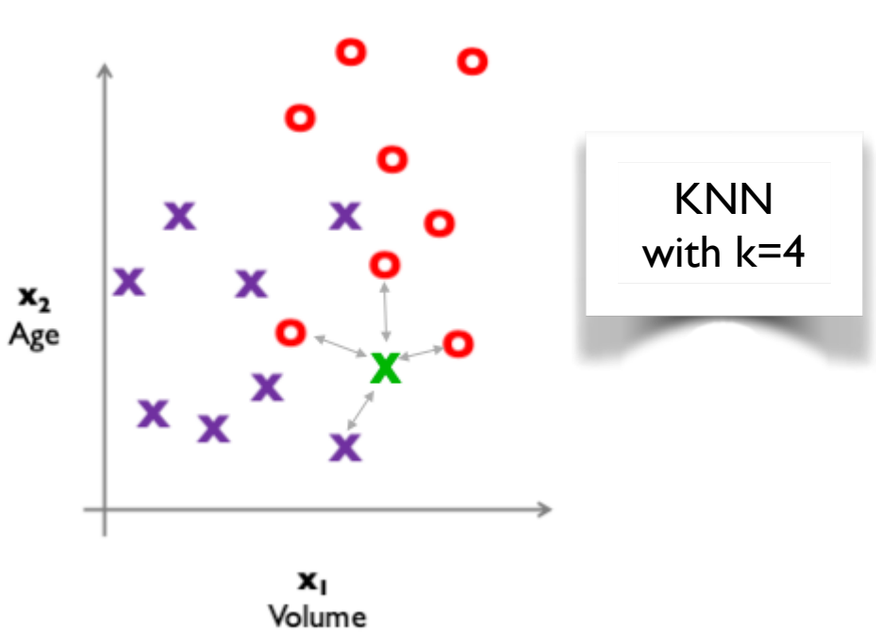
Critics *about k-nn*

1. *What kind of distance to use?*
2. *What is the best value for k?*
3. *Are we guaranteed to minimise the classification errors?*
4. *What if we have unbalanced training sets?* *(for example 10x more data for class a than class b)*
    - *We probably give priority to the class with lots of points*
    - *Is it bad or good?*

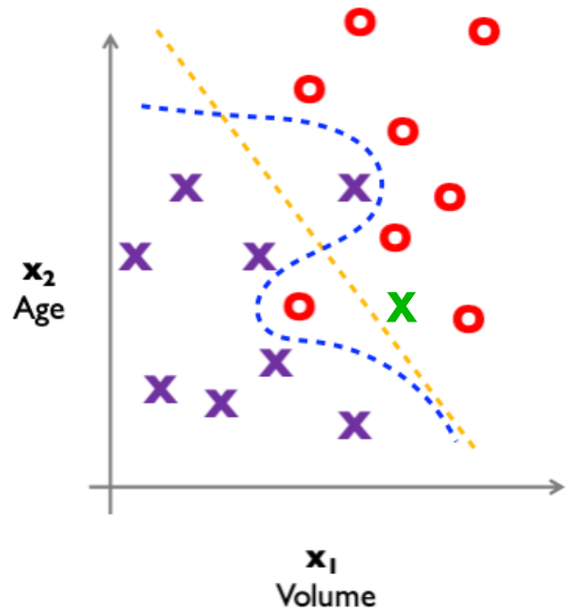
Instance-based vs model-based learning

Instance-based learning: the system learns the examples by heart and generalises by similarity

Model-based learning: the system learns a mapping function $\hat{y} = h(\mathbf{x})$ defined by an equation and a set $\{\theta\}$ of parameters



KNN
with k=4

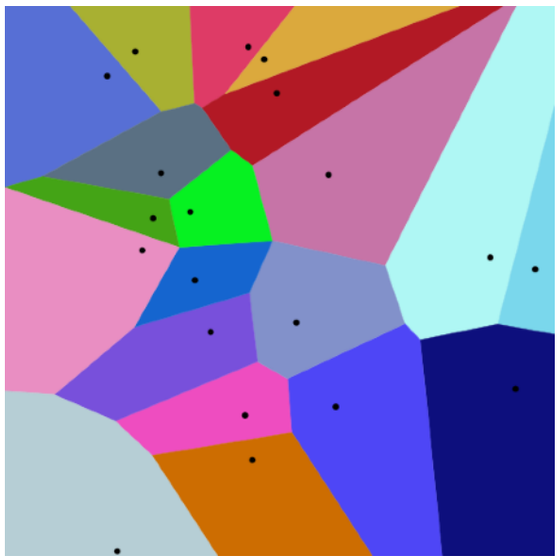


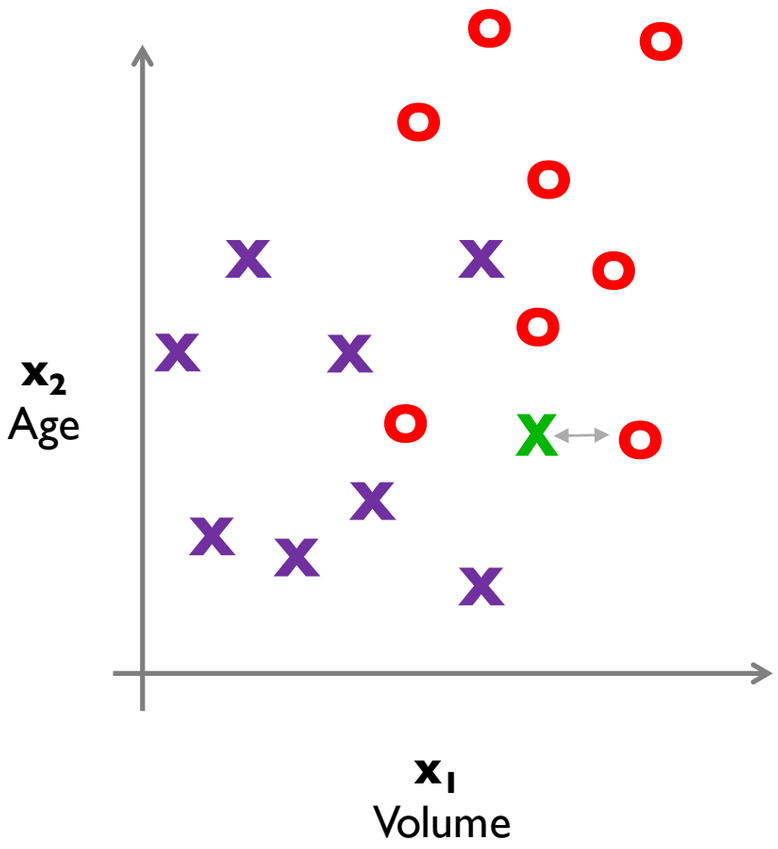
Logistic regression with a linear model (yellow) and a non-linear model (blue)

- The KNN is an instance-based learning approach

1-nn

- k-nn with k=1
- Predict the same value/class as the nearest instance in the training set
- We can visualise the partition regions of points “belonging” to a training point. This is called a **Voronoi diagram**





Assuming N examples in the training set, what are the temporal (cpu time) and spatial (memory) complexity of K-NN?

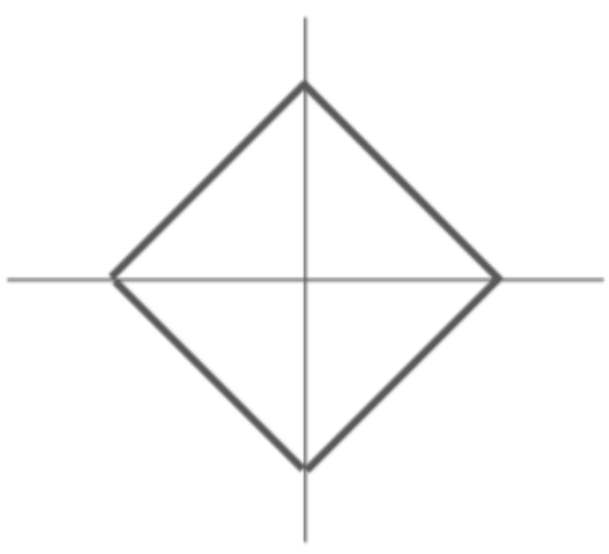
Activity

- At training time?
- For 1 prediction?
- Are these complexities good or bad?

Distance metrics to use?

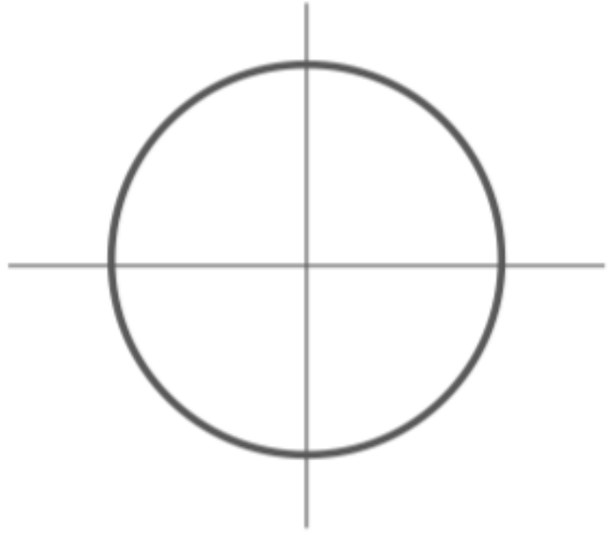
L1 (Manhattan) distance

$$d_1(I_1, I_2) = \sum_p |I_1^p - I_2^p|$$



L2 (Euclidean) distance

$$d_2(I_1, I_2) = \sqrt{\sum_p \left(I_1^p - I_2^p\right)^2}$$



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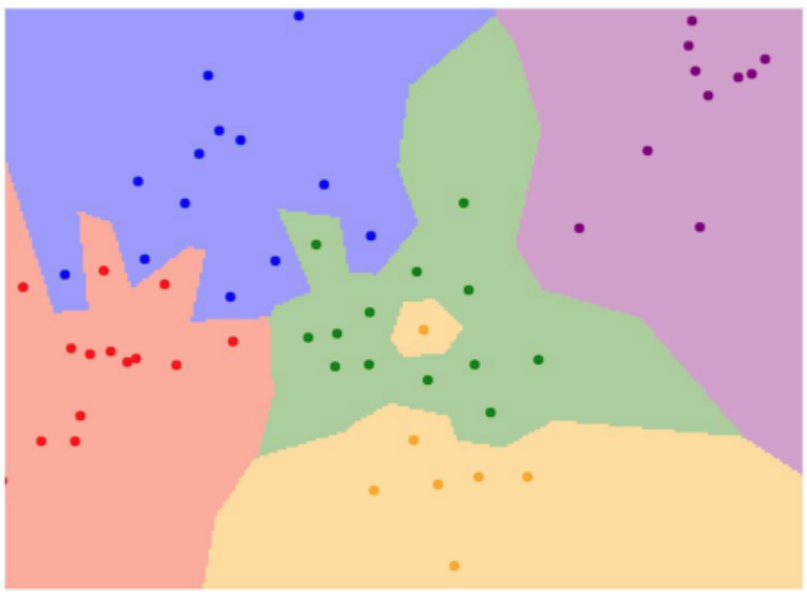
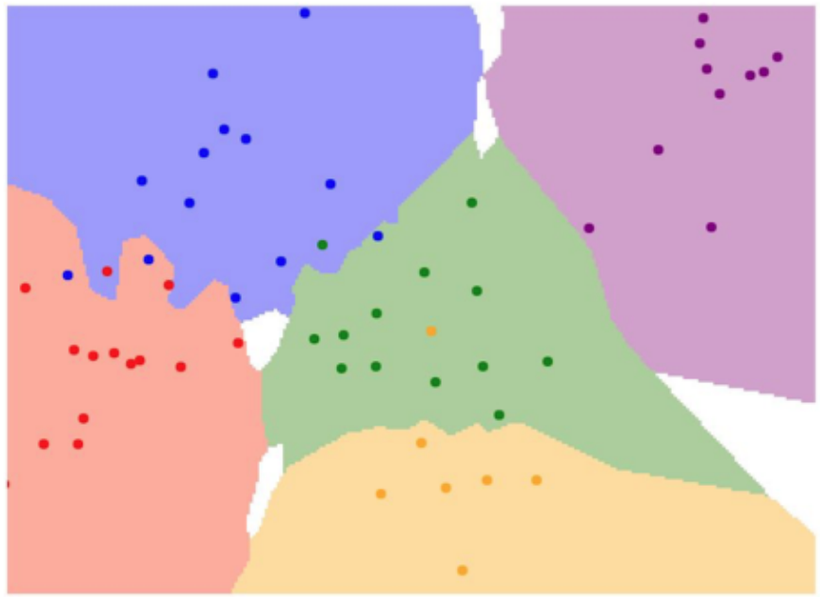
1-nn vs. k-nn

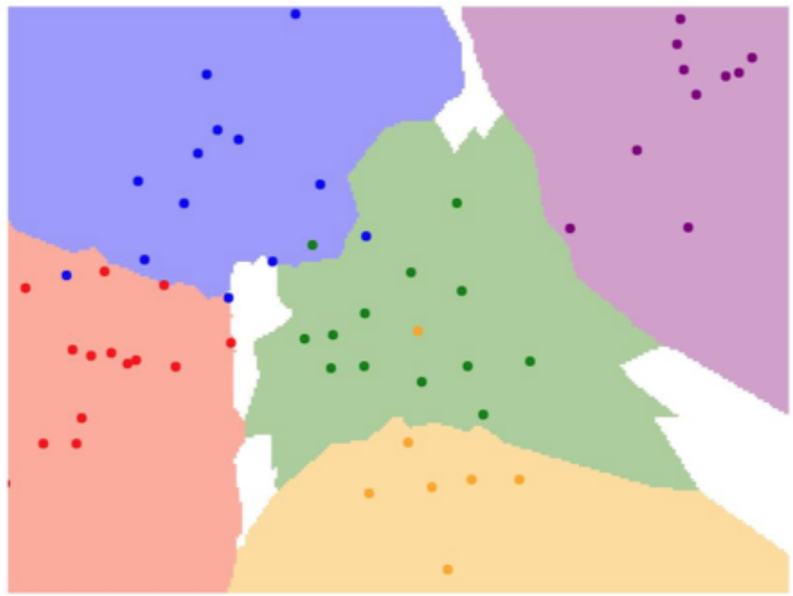
- Larger k brings some advantages
  - More confidence, especially with noisy data
  - Provides “probabilistic” information
    - The ratio of examples for each class gives information about the confidence or ambiguity of the decision
- However, too large values of k may be detrimental
  - It destroys the locality of the estimation since farther examples are taken into account
  - It increases the computational burden



K = 1



K = 3



K = 5

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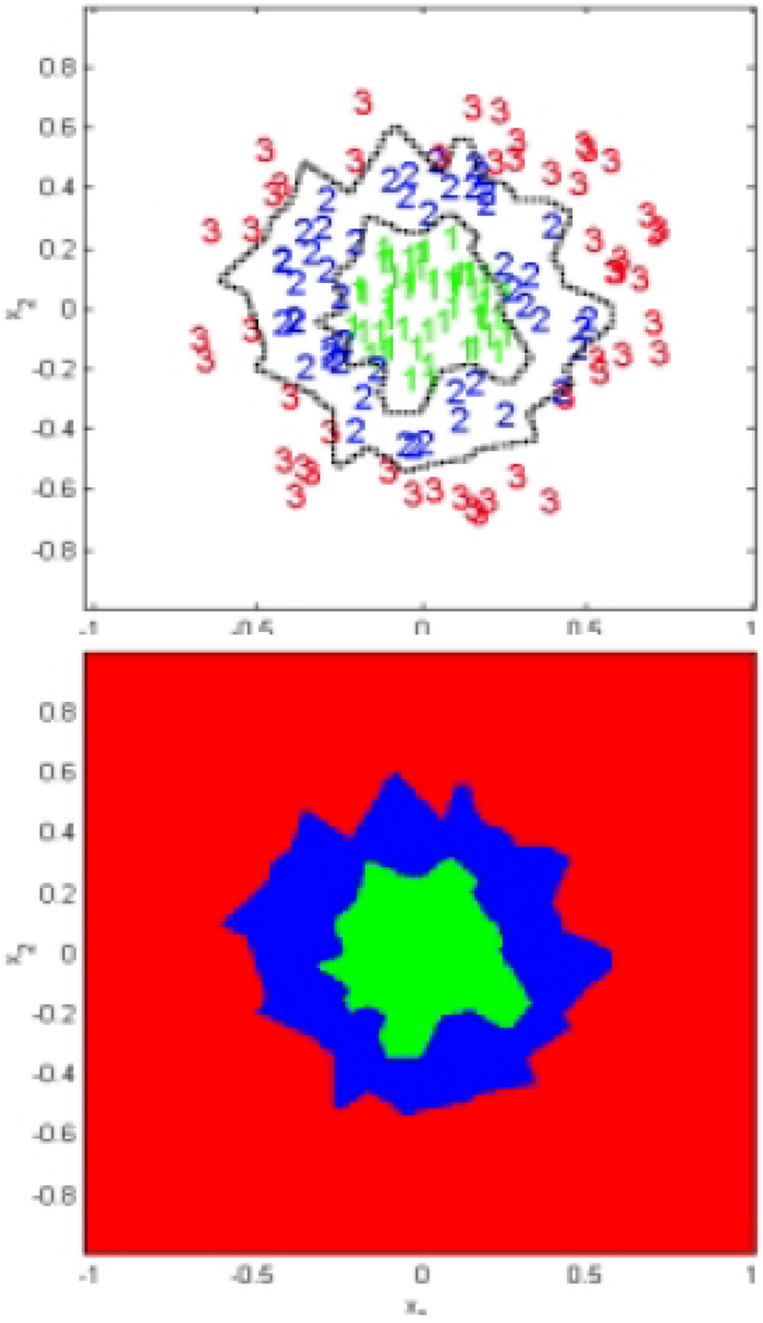
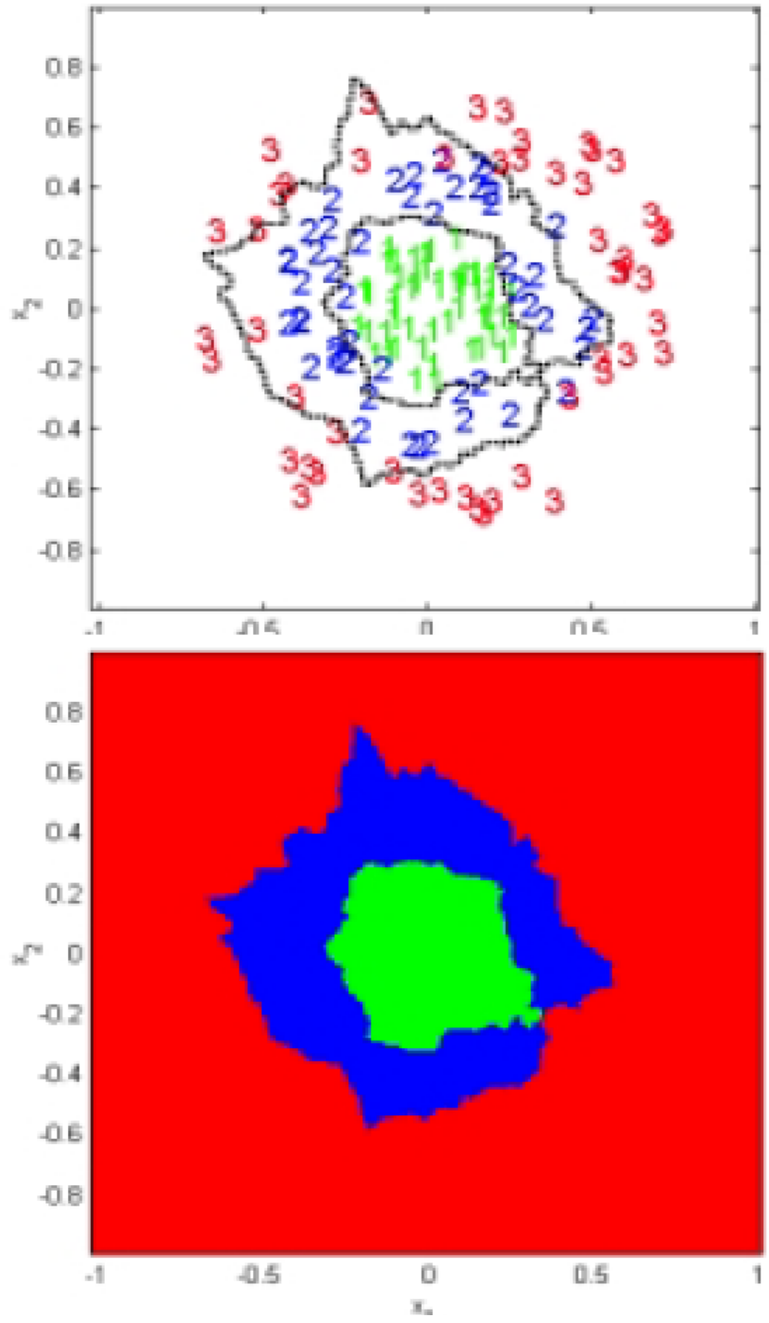
Check out the live demo under http://vision.stanford.edu/teaching/cs231n-demos/knn/

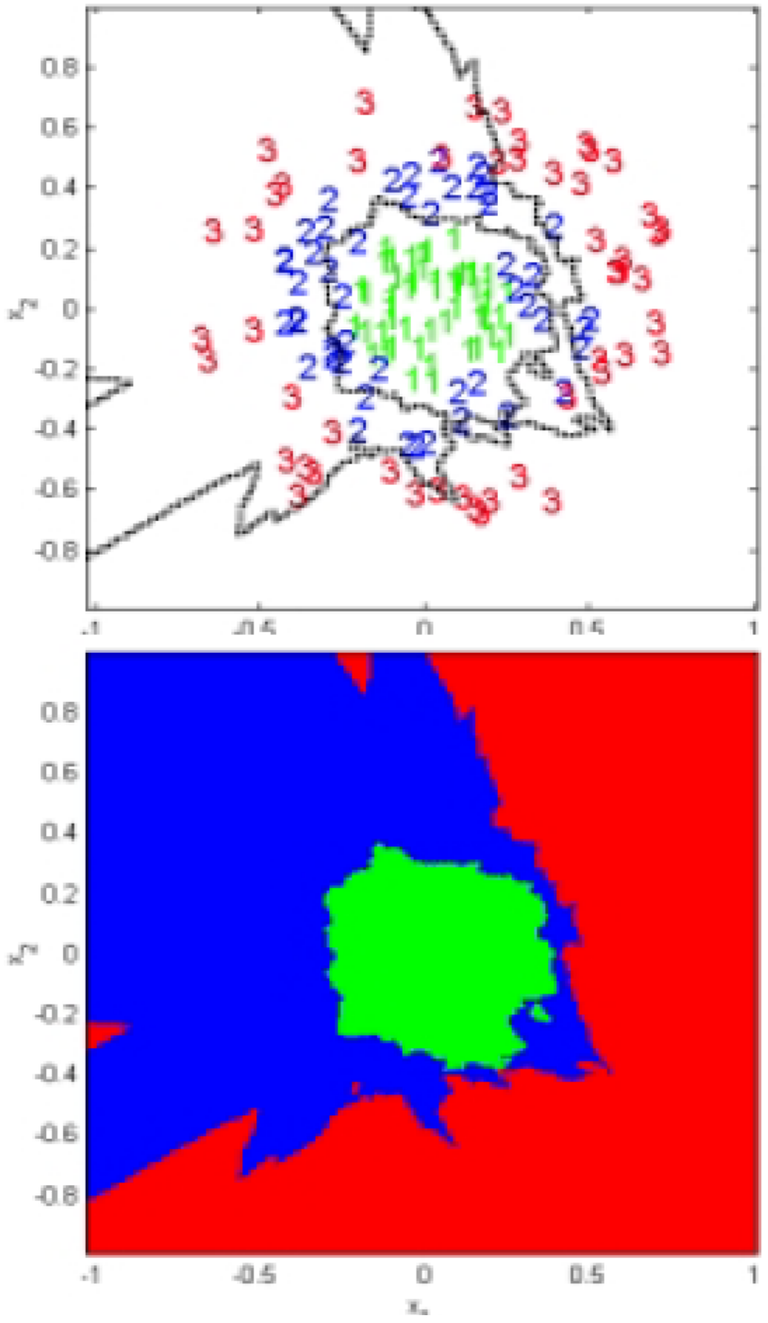
k=1



k=5



k=20



Integer values (and colours) indicate class labels.

k-nn hyperparameters to tune

- Hyper-parameters to be tuned
  - **normalisation type**: none, min-max rescaling, zero-norm[1]
  - **distance metric**: Euclidian, Manhattan, Mahalanobis, …
  - **k**: from 1 to …
  - **strategies in case of no majority**: min distance class, go to k+1, …
- k-nn is heavy in terms of
  - **memory**: the full training set needs to be stored and accessible
  - **cpu**: the distance is computed against the whole training set O(N)
    - some optimisation techniques can be used such as k-d tree

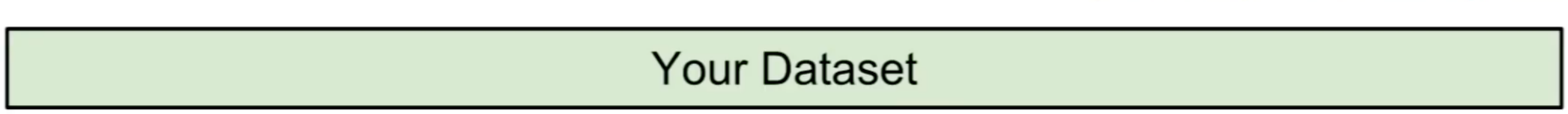
(1) See chapter on data preparation in few weeks to a full range of potential normalisations

k-nn tuning - hyper parameters tuning

Setting Hyperparameters

Idea #1: Choose hyperparameters that work best on the data

BAD: K = 1 always works perfectly on training data



Idea #2: Split data into **train** and **test**, choose hyperparameters that work best on test data

BAD: No idea how algorithm will perform on new data

Idea #3: Split data into **train**, **val**, and **test**; choose hyperparameters on val and evaluate on test

Better!

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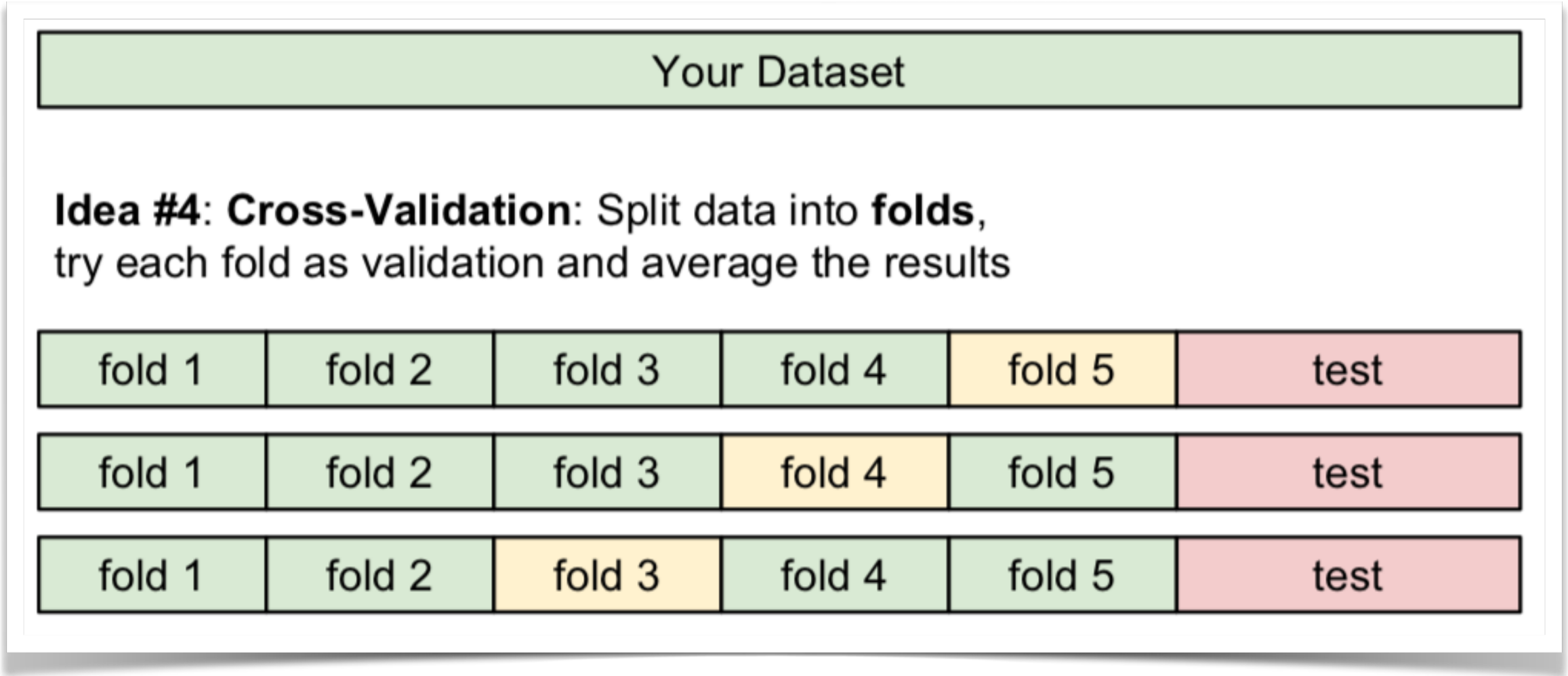
k-nn tuning - hyper parameters tuning



ML Engineering tip: never do idea 1, do at least idea 2, even better if you do idea 3.
In case of small data sets, do idea 4 and observe the variability of your performances.

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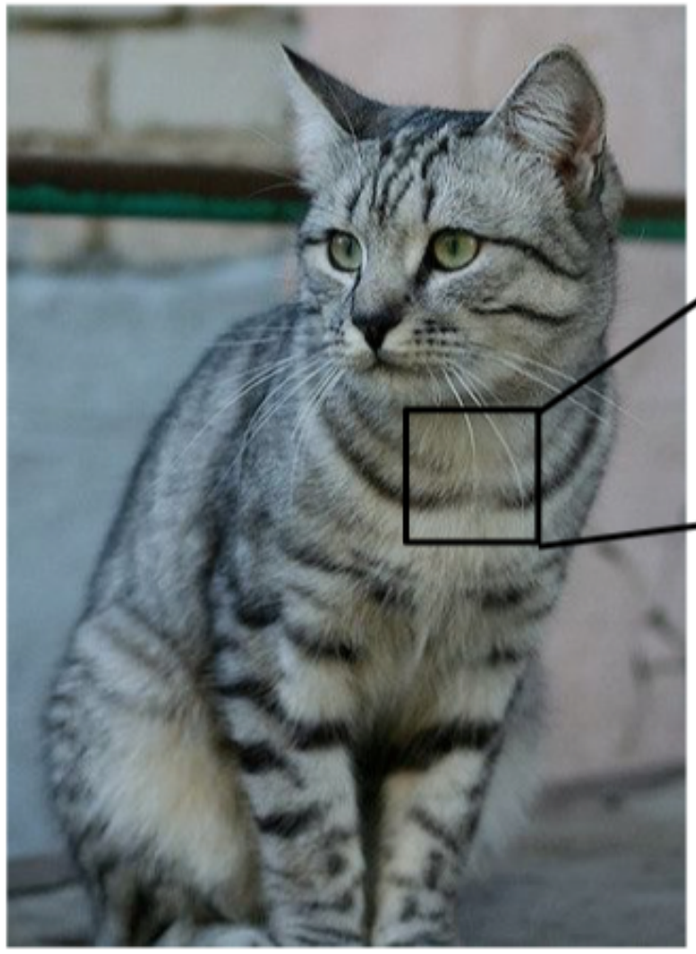
2.3 Use case: k-nn for image classification

By Balu Ertl https://upload.wikimedia.org/wikipedia/commons/5/54/Euclidean_Voronoi_diagram.svg

Some preliminary questions

- How to compute image distances?
- What metric to use?
- Is using KNN a good idea for image classification?
  - If no, why?
  - If yes, in which conditions?

Image representation




```
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 [ 91  98 102 106 104  79  98 103  99 105 123 136 110 105  94  85]
 [ 76  85  90 105 128 105  87  96  95  99 115 112 106 103  99  85]
 [ 99  81  81  93 120 131 127 100  95  98 102  99  96  93 101  94]
 [106  91  61  64  69  91  88  85 101 107 109  98  75  84  96  95]
 [114 108  85  55  55  69  64  54  64  87 112 129  98  74  84  91]
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 [ 89  93  90  97 108 147 131 118 113 114 113 109 106  95  77  80]
 [ 63  77  86  81  77  79 102 123 117 115 117 125 125 130 115  87]
 [ 62  65  82  89  78  71  80 101 124 126 119 101 107 114 131 119]
 [ 63  65  75  88  89  71  62  81 120 138 135 105  81  98 110 118]
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 [122 121 102  80  82  86  94 117 145 148 153 102  58  78  92 107]
 [122 164 148 103  71  56  78  83  93 103 119 139 102  61  69  84]]
```
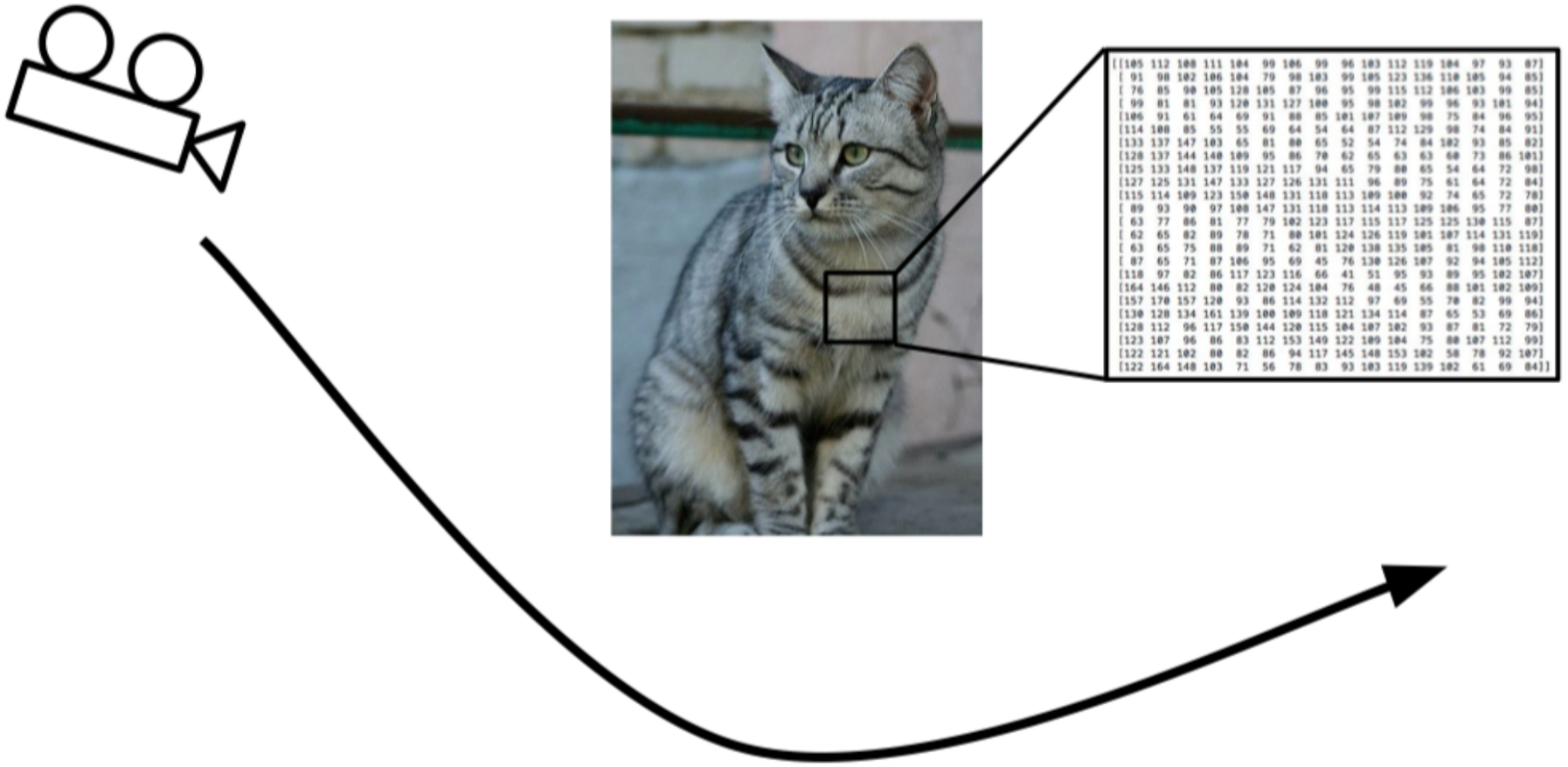

What the computer sees

An image is just a big grid of numbers between [0, 255]:

e.g. 800 x 600 x 3
(3 channels RGB)

Challenges: viewpoint



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Challenges: illumination / deformations

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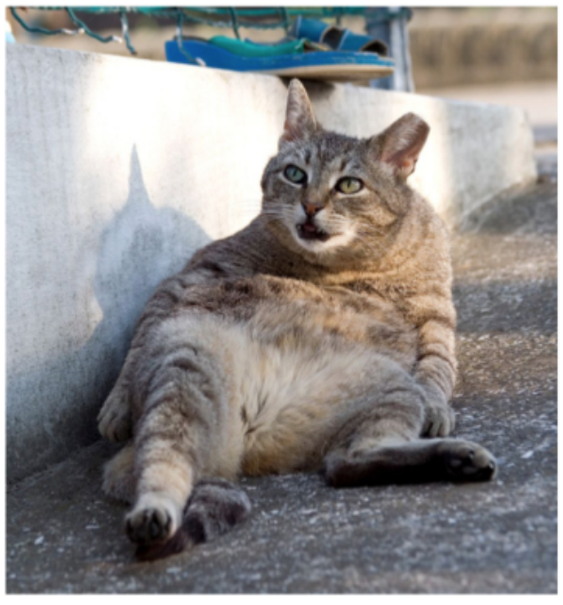

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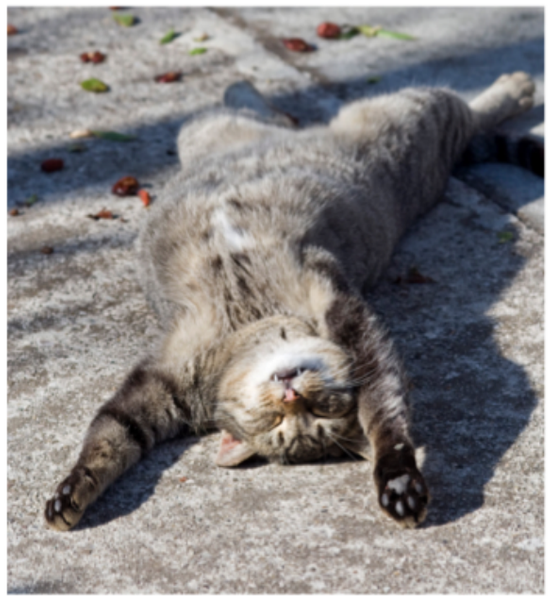

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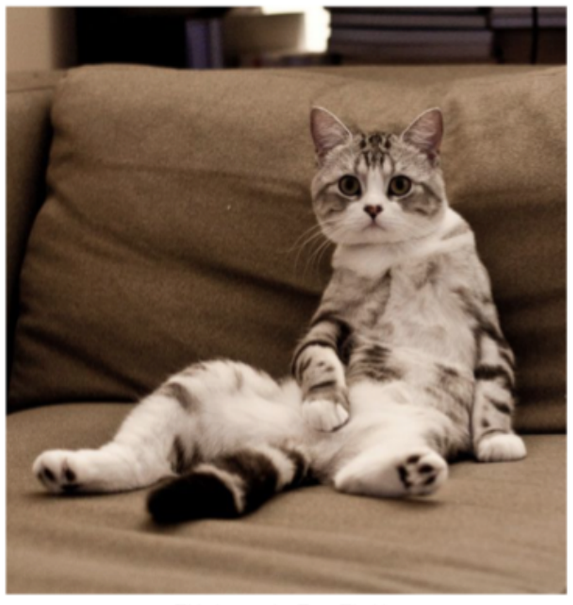

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Challenges: occlusions / background

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Challenges: intra-class variabilities

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Machine learning approach with KNN

```
def train(images, labels):
  # Machine learning!
  return model
```

→ Memorize all data and labels

```
def predict(model, test_images):
  # Use model to predict labels
  return test_labels
```

→ Predict the label of the most similar training image

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Let's assume we use an L1 distance metric

L1 distance: $$d_1(I_1, I_2) = \sum_p |I_1^p - I_2^p|$$

test image

56	32	10	18
90	23	128	133
24	26	178	200
2	0	255	220

\-

training image

10	20	24	17
8	10	89	100
12	16	178	170
4	32	233	112

=

pixel-wise absolute value differences

46	12	14	1
82	13	39	33
12	10	0	30
2	32	22	108

add → 456

L2 (Euclidian) could also be appropriate depending to the type of images.

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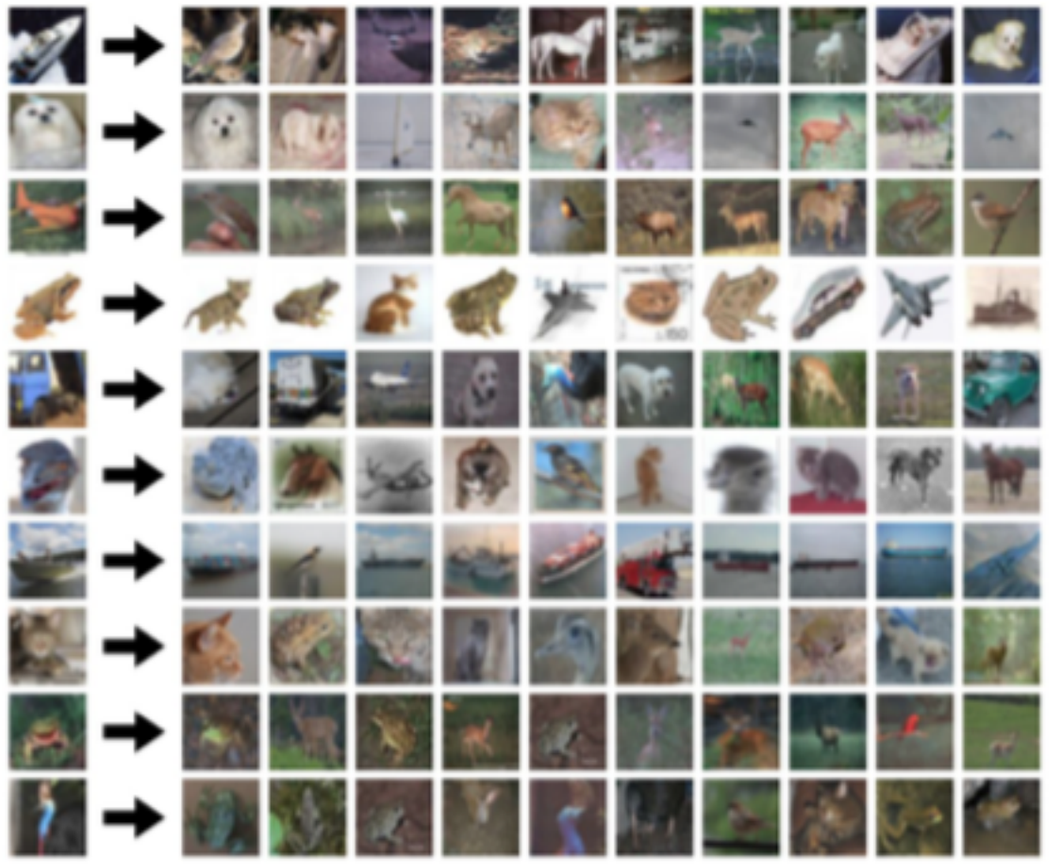
Example on CIFAR10

10 classes
50,000 training images
10,000 testing images

Test images and nearest neighbors



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Nearest Neighbor classifier

```python
import numpy as np

class NearestNeighbor:
  def __init__(self):
    pass

  def train(self, X, y):
    """ X is N x D where each row is an example. Y is 1-dimension of size N """
    # the nearest neighbor classifier simply remembers all the training data
    self.Xtr = X
    self.ytr = y

  def predict(self, X):
    """ X is N x D where each row is an example we wish to predict label for """
    num_test = X.shape[0]
    # lets make sure that the output type matches the input type
    Ypred = np.zeros(num_test, dtype = self.ytr.dtype)

    # loop over all test rows
    for i in xrange(num_test):
      # find the nearest training image to the i'th test image
      # using the L1 distance (sum of absolute value differences)
      distances = np.sum(np.abs(self.Xtr - X[i,:]), axis = 1)
      min_index = np.argmin(distances) # get the index with smallest distance
      Ypred[i] = self.ytr[min_index] # predict the label of the nearest example

    return Ypred
```

Memorize training data

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Nearest Neighbor classifier

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      min_index = np.argmin(distances) # get the index with smallest distance
      Ypred[i] = self.ytr[min_index] # predict the label of the nearest example

    return Ypred
```

For each test image:
Find closest train image
Predict label of nearest image

argmin returns the index of the minimum value in distances

Broadcasting is used here. See Ex 1 of PW-02

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Classification results

Nearest neighbours

About 30% accuracy on 10 classes

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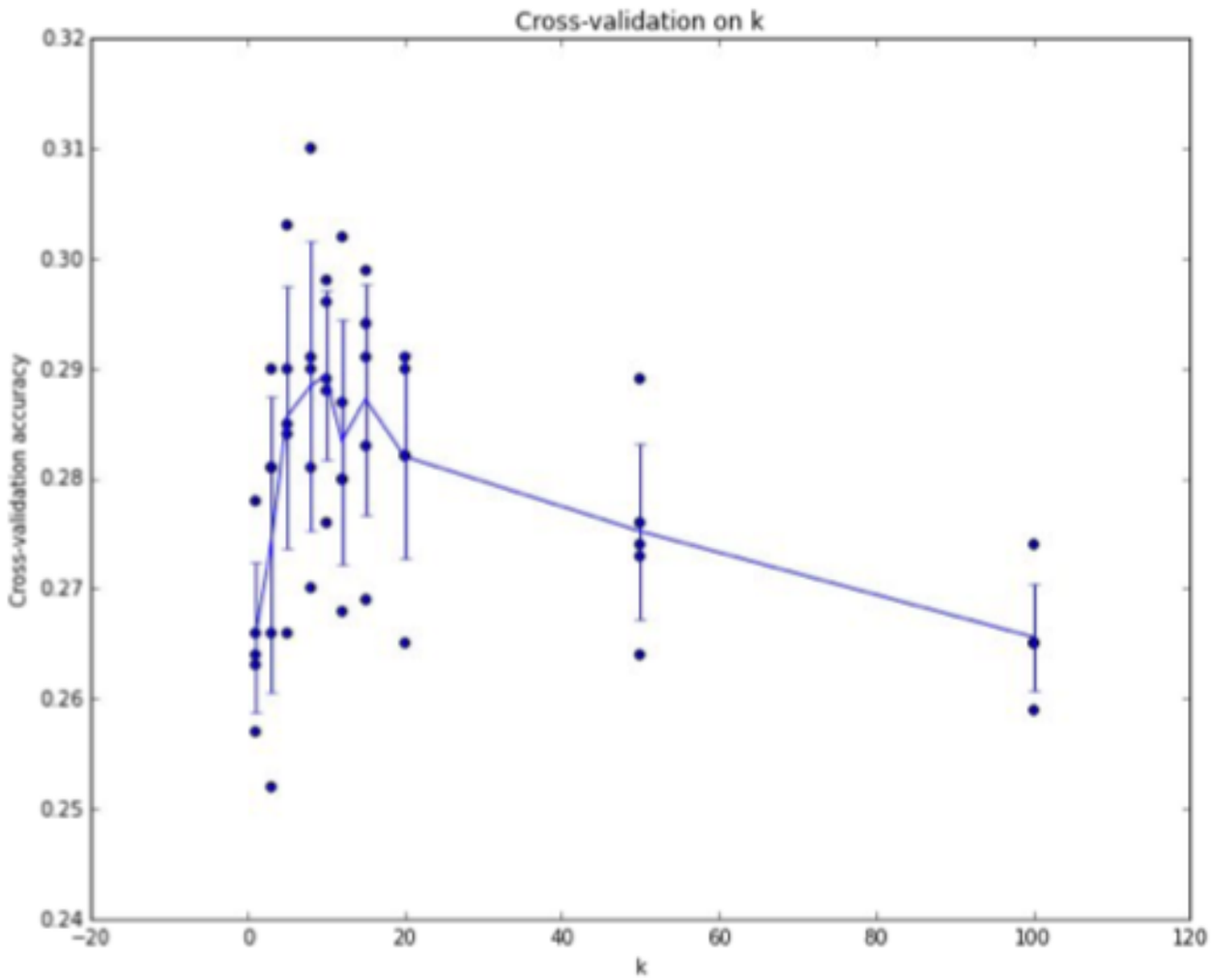
Setting Hyperparameters



Example of
5-fold cross-validation
for the value of **k.**

Each point: single outcome.

The line goes through the mean, bars indicated standard deviation

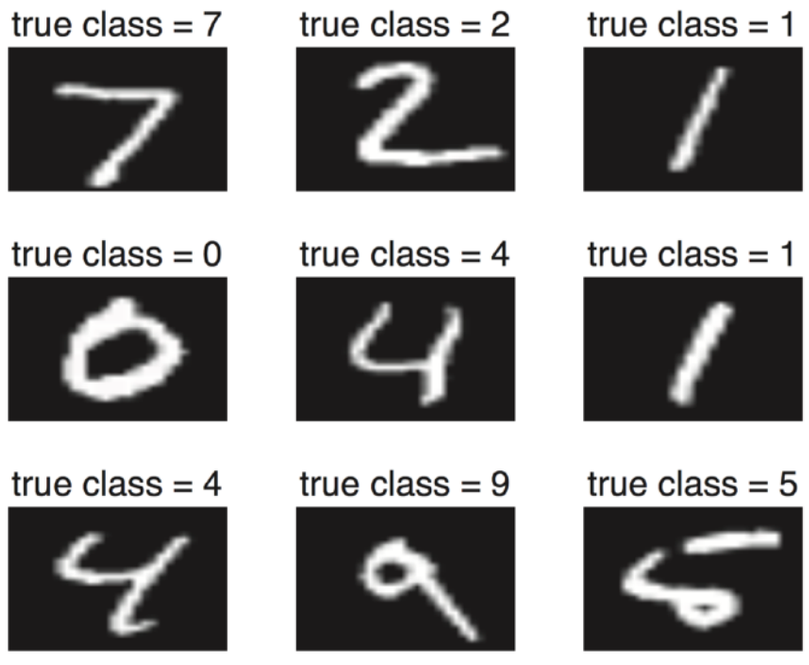
(Seems that k ~= 7 works best for this data)

About 30% accuracy on 10 classes. In practice KNN is a bad idea on images with high variabilities.

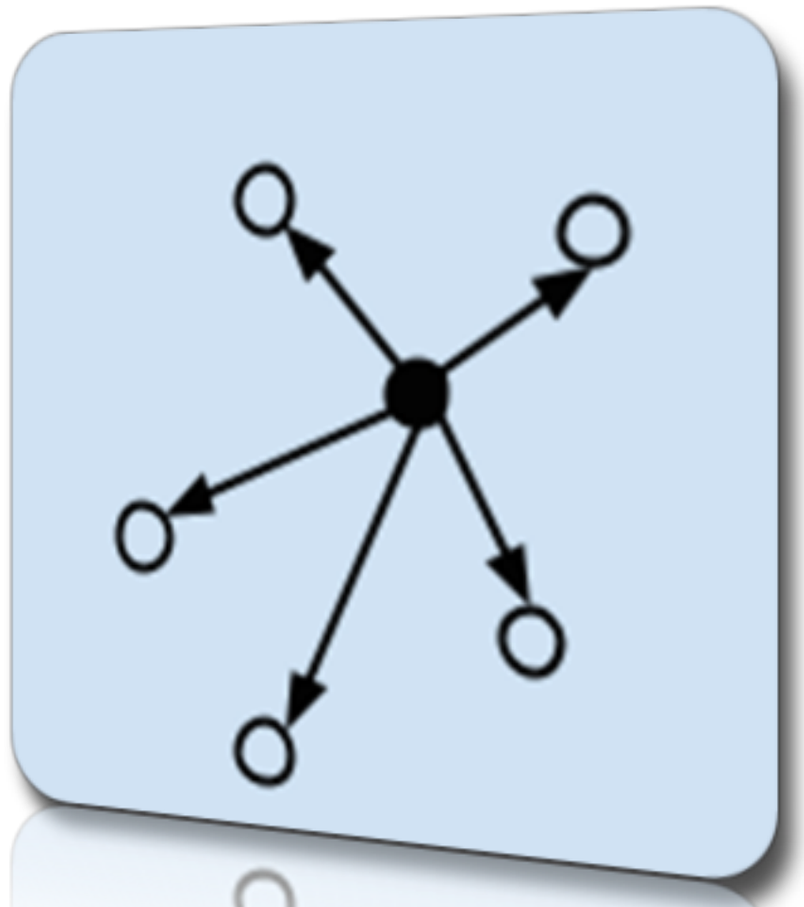
KNN on MNIST handwritten digits images

Activity

- KNN shows decent performances on this dataset, above 90% accuracy.
  - Why? State several reasons.



2.4 Regressor KNN



What is it?

How to use it?

KNN Regressor

The **k-nearest regressor** algorithm is a method that predicts a target value $\hat{y}$ based on the $\{y_k\}_K$ values of the K closest examples in the training set.

- We could opt for a simple average of the y_k values with

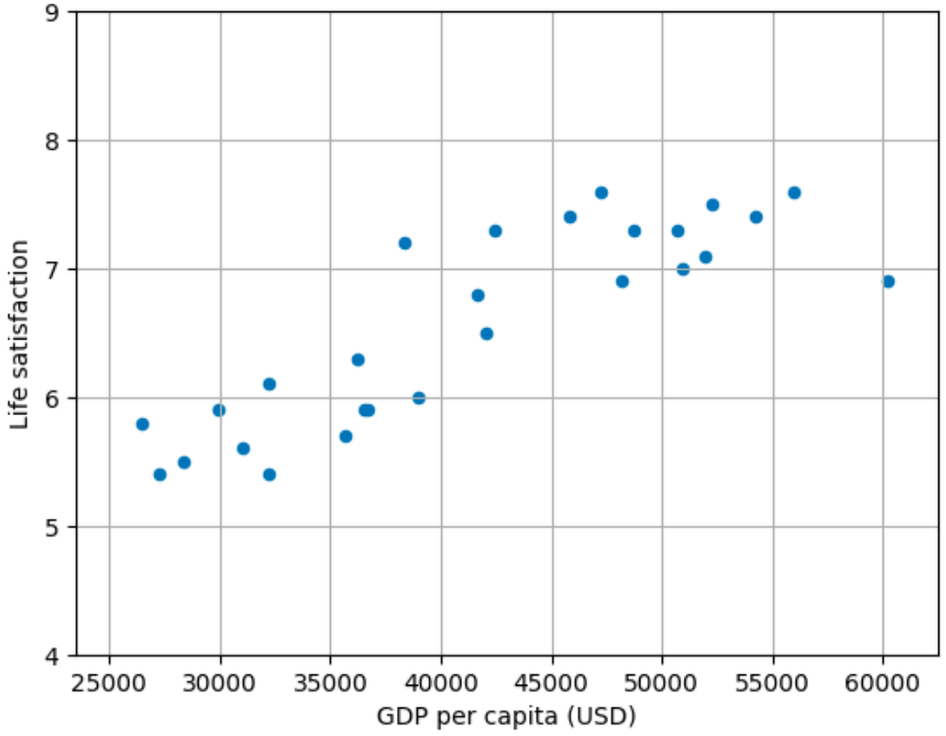
  $\hat{y} = \frac{1}{K}\sum_{k=1}^{K} y_k$, where each y_k are corresponding to the k-nearest neighbour.

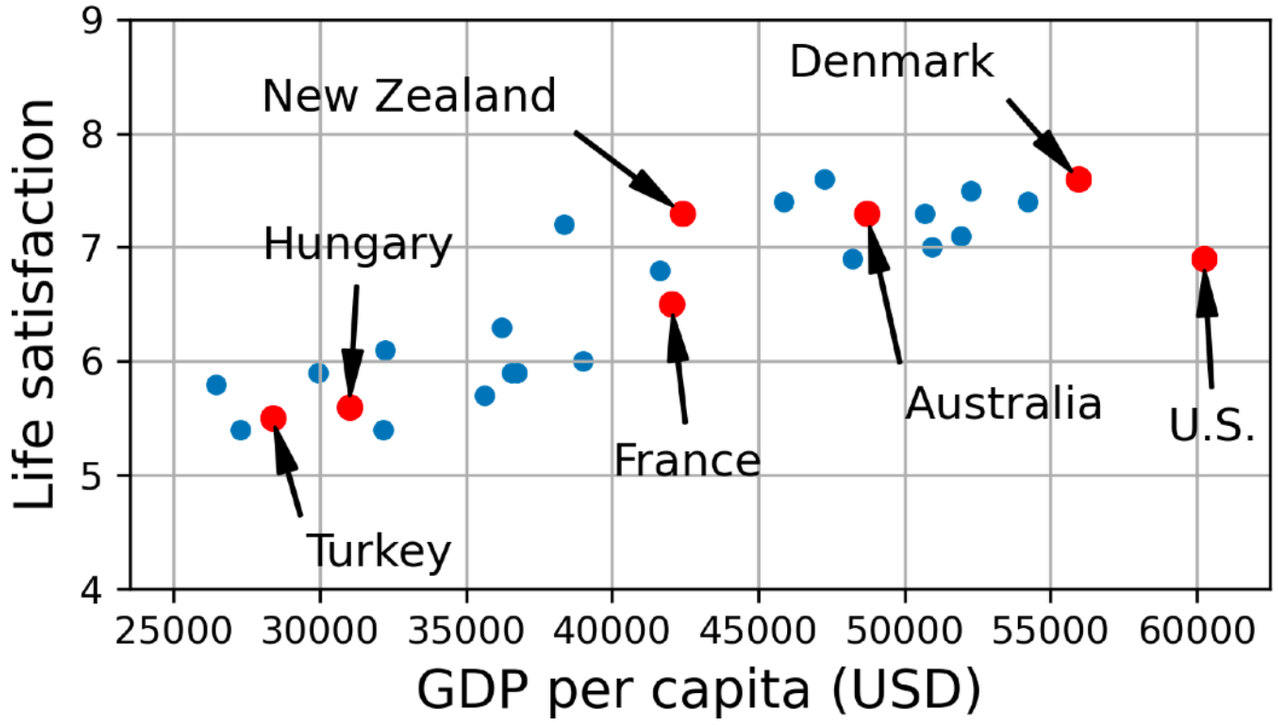
- Other strategies apply, e.g. using a weighted average where the weights are decreasing either with the rank :

  $\hat{y} = \sum_{k=1}^{K} w_k y_k$, with e.g. $\{w_1 < w_2 < \ldots < w_K\}$ and $\sum_{k=1}^{K} w_k = 1.0$

  or with the inverse of the distance to the nearest point $w_k \propto \frac{1}{d(x, x_k)}$

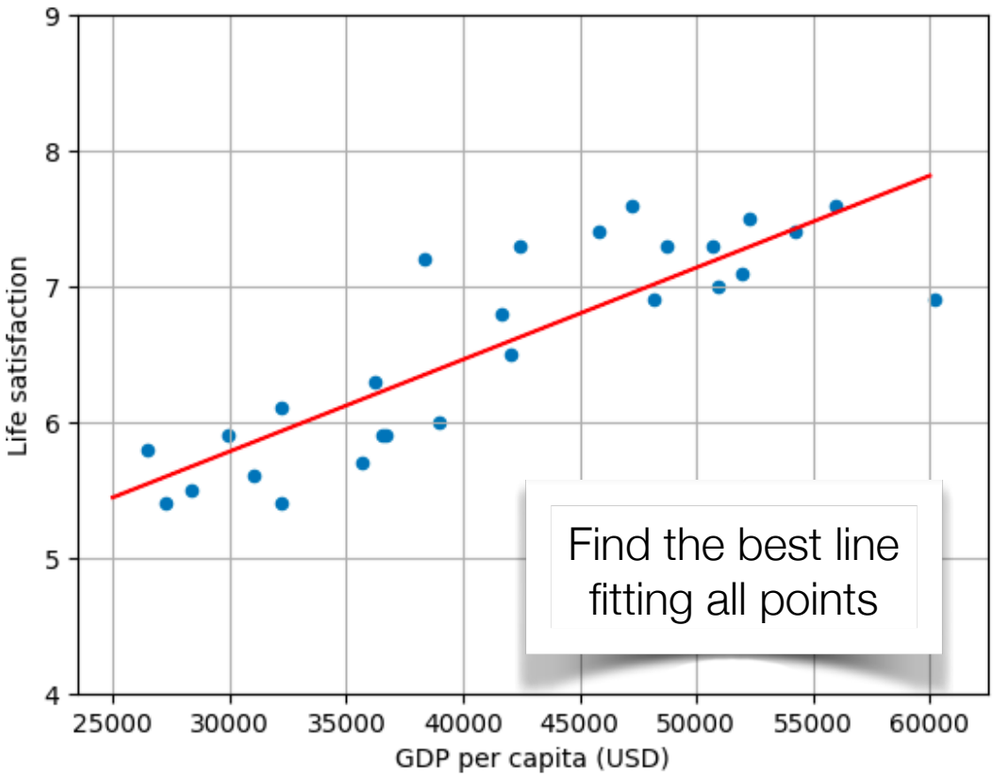
Example: more $$$ = happiness ?

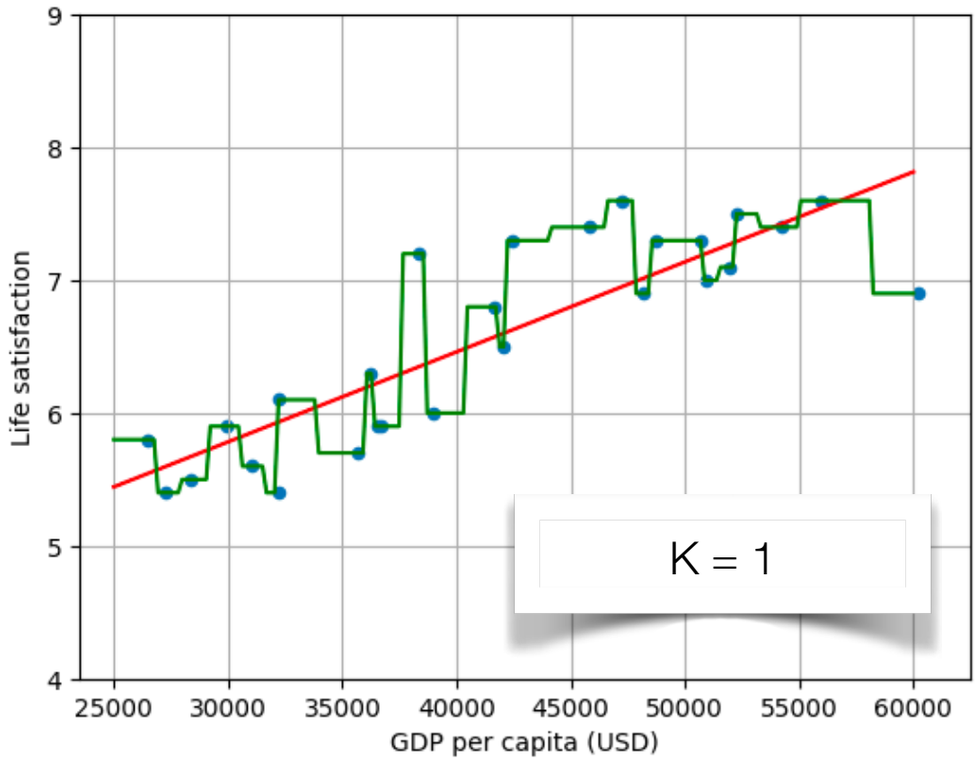




- Source: https://ourworldindata.org/grapher/gdp-vs-happiness
- In x: the GDP = gross domestic product, a measure of the goods and services produced in a given country

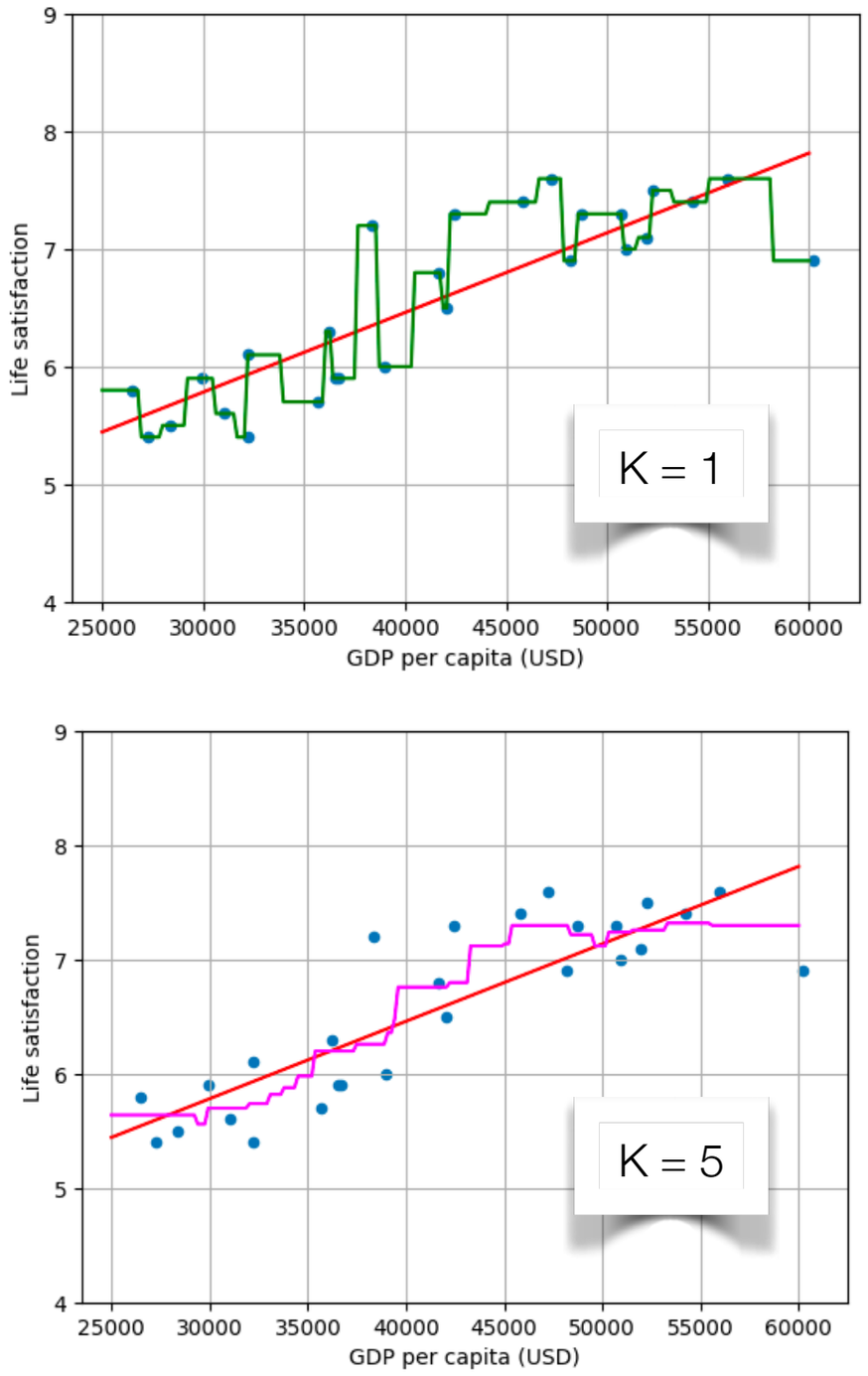
Linear regression vs K-NN regression

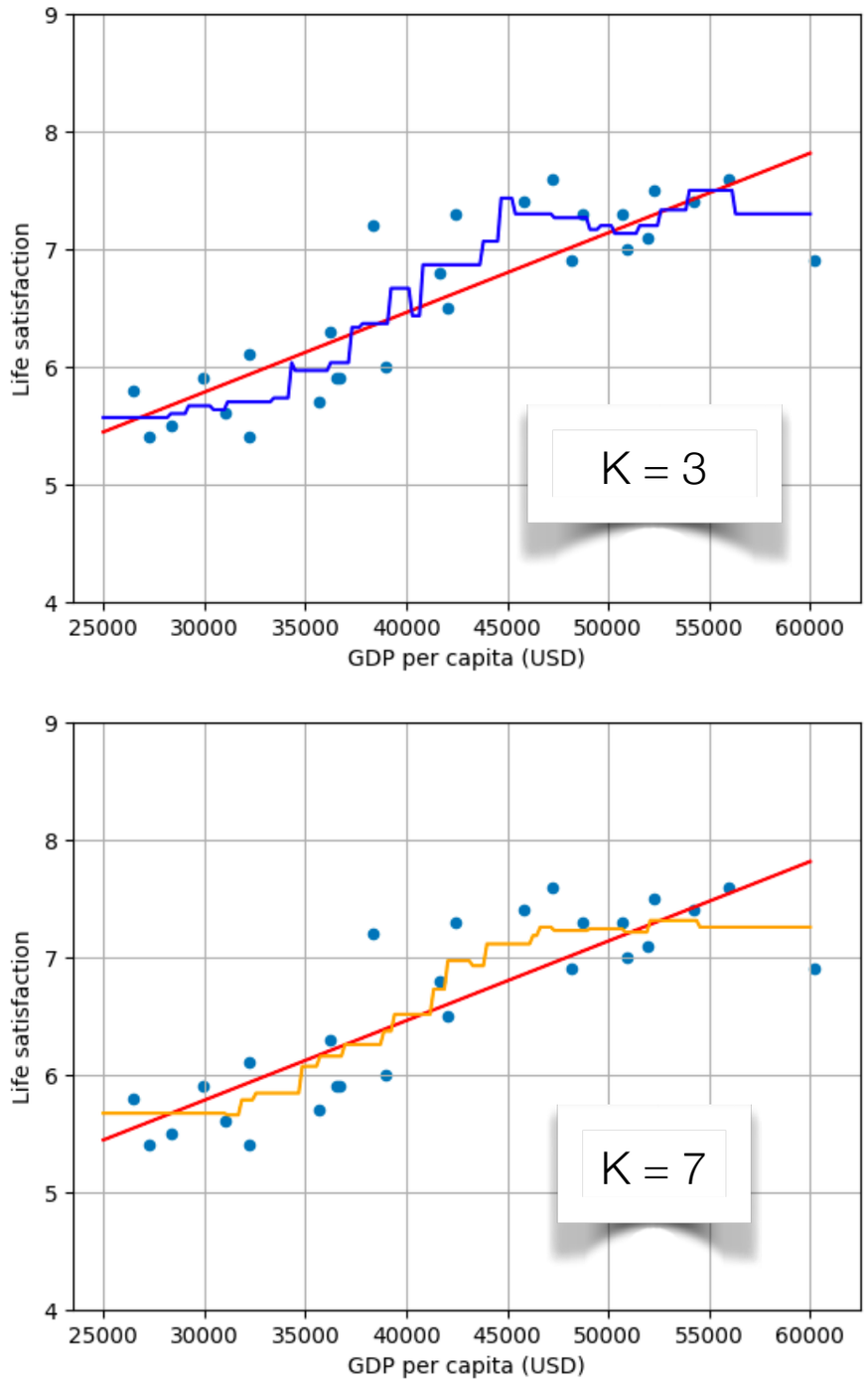




- On the left, we used the linear regression algorithm that finds the equation $\hat{y} = \theta_0 + \theta_1 x$ by minimising the least square errors between the line and the input points.
  - We will re-visit linear regression soon!

Increasing K





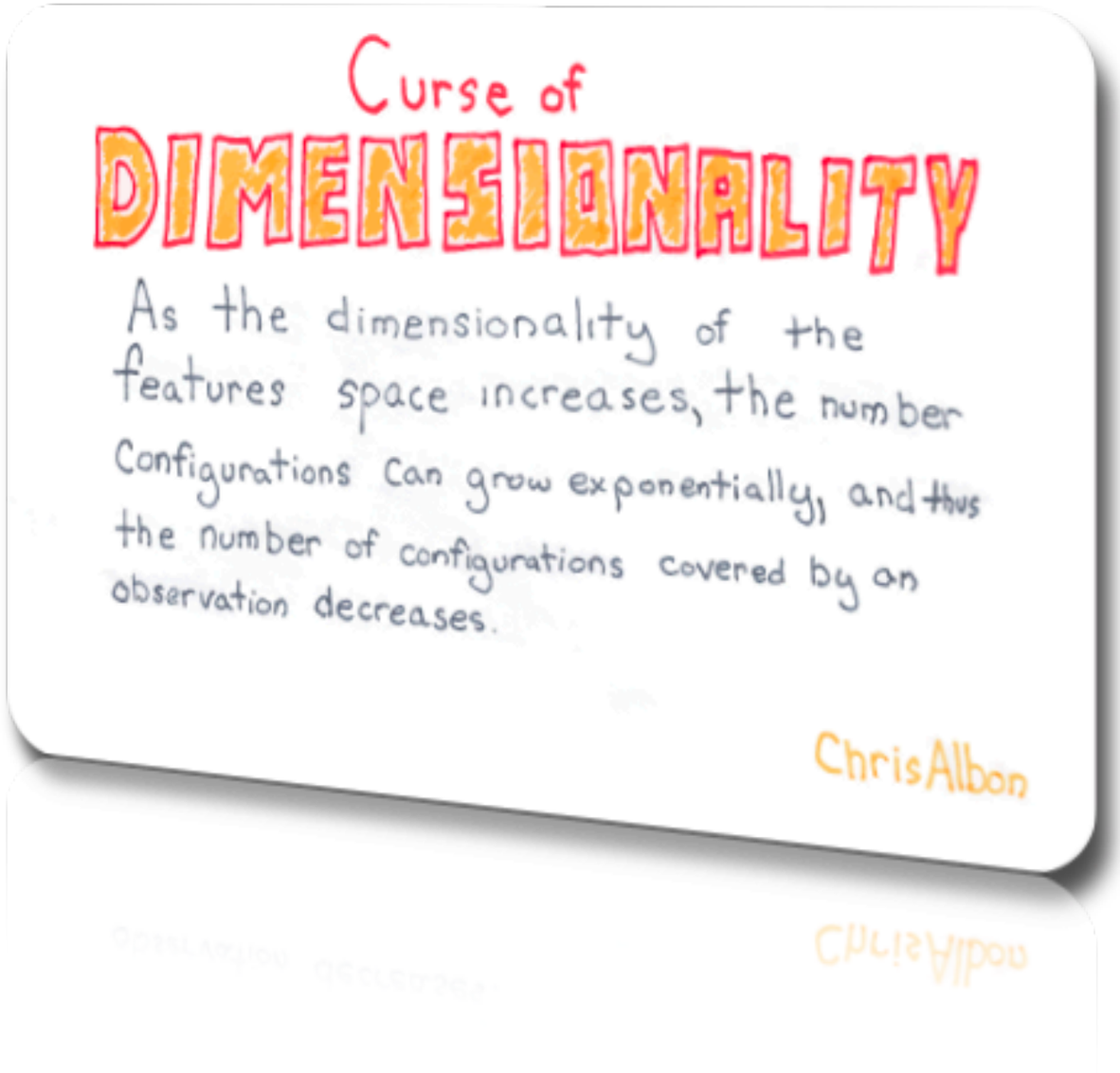
- Higher K brings smoothness

2.5 The curse of dimensionality

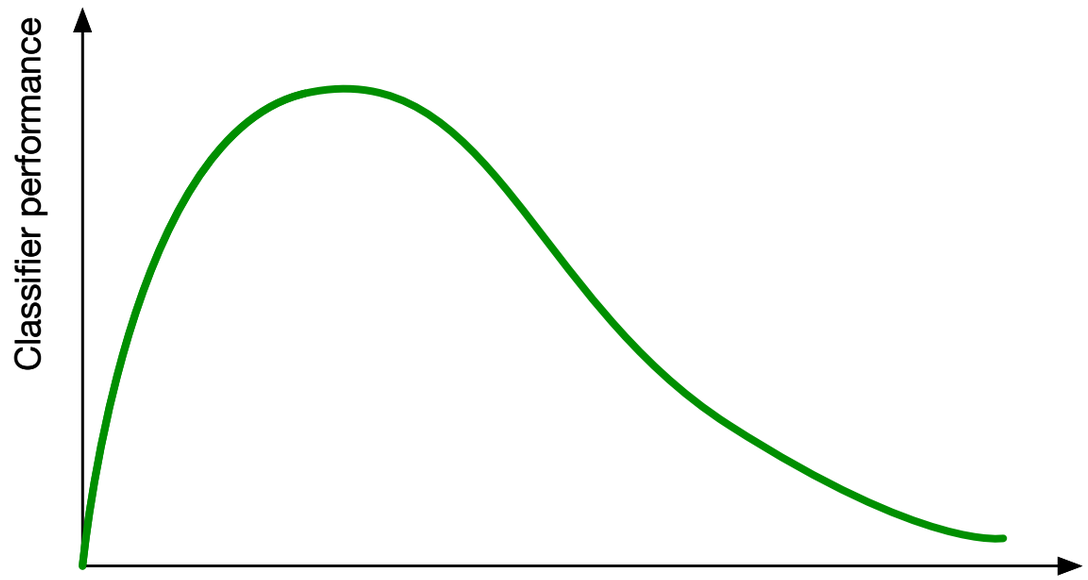
What is it?

Why that?

Does it impact k-nn?



Curse of dimensionality - what is it?

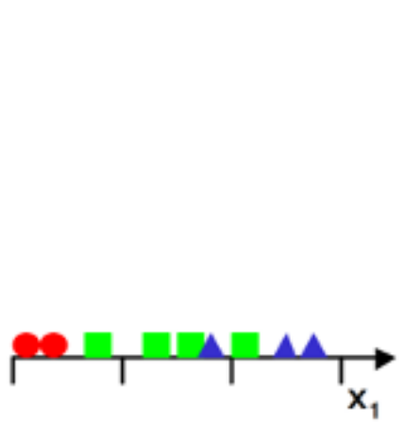


ML Engineering tip: adding features typically increases the performance

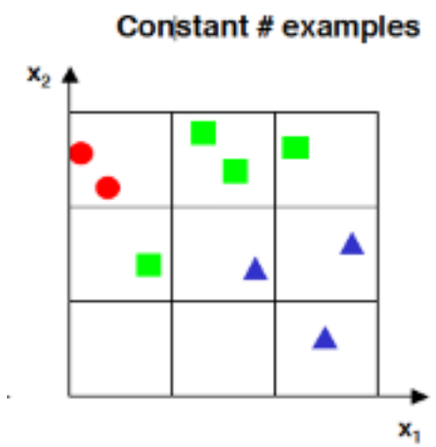
- Yes, having extra information (features) usually helps
- However, we often observe a decrease of performances when inserting more features

The **curse of dimensionality** is when we observe a decrease of performance when increasing the number of features. This is due to the lack of samples N with respect to the dimensions D of the input space.

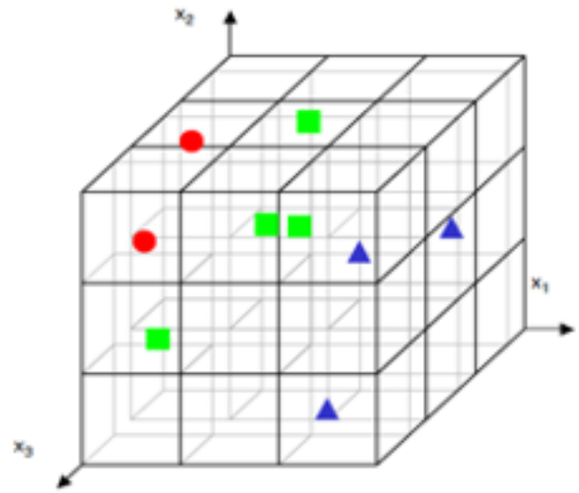
Curse of dimensionality - why that?



D=1
3 regions



D=2
9 regions



D=3
27 regions

… 3^D regions

- Data sparsity occurs when moving to higher dimensions.
- The volume of the space (the number of regions) grows exponentially with the number of features.

Revised **ML Engineering tip**: adding features typically increases the performance, up to a certain point where the curse of dimensionality impacts the performance.

Curse of dimensionality - impact on k-nn

- Distance-based classifiers as k-nn are impacted by the curse of dimensionality
  - The distance is indeed computed considering the D dimensions of the features
- Side note: a decrease of performance when inserting more features could also be the result of:
  - Noisy features
  - Redundant features
  - Un-normalized features
- Using k-nn often involves **feature selection** and well-thought **normalisation** procedures[1]

(1) Stay tuned and visit chapter on data preparation in few weeks to a full range of potential normalisations

Conclusions on K-NN

- K-NN is an instance-based approach - vs a model-based approach
  - Quite bad in terms of cpu at inference time
- Simple, intuitive **supervised classification** algorithm
  - Find the k nearest neighbours in the training set
  - Predict the label according to a majority vote on the neighbours
- Can also be used to perform **supervised regression**
  - Find the k nearest neighbours in the training set
  - Predict the value according to, e.g. the averaged y values of the neighbours
- Distance metric and K are **hyperparameters**
- Choosing hyperparameters using the training set through a **validation** or **cross-validation** procedure is a good idea
- Beware of the **curse of dimensionality** when using k-nn