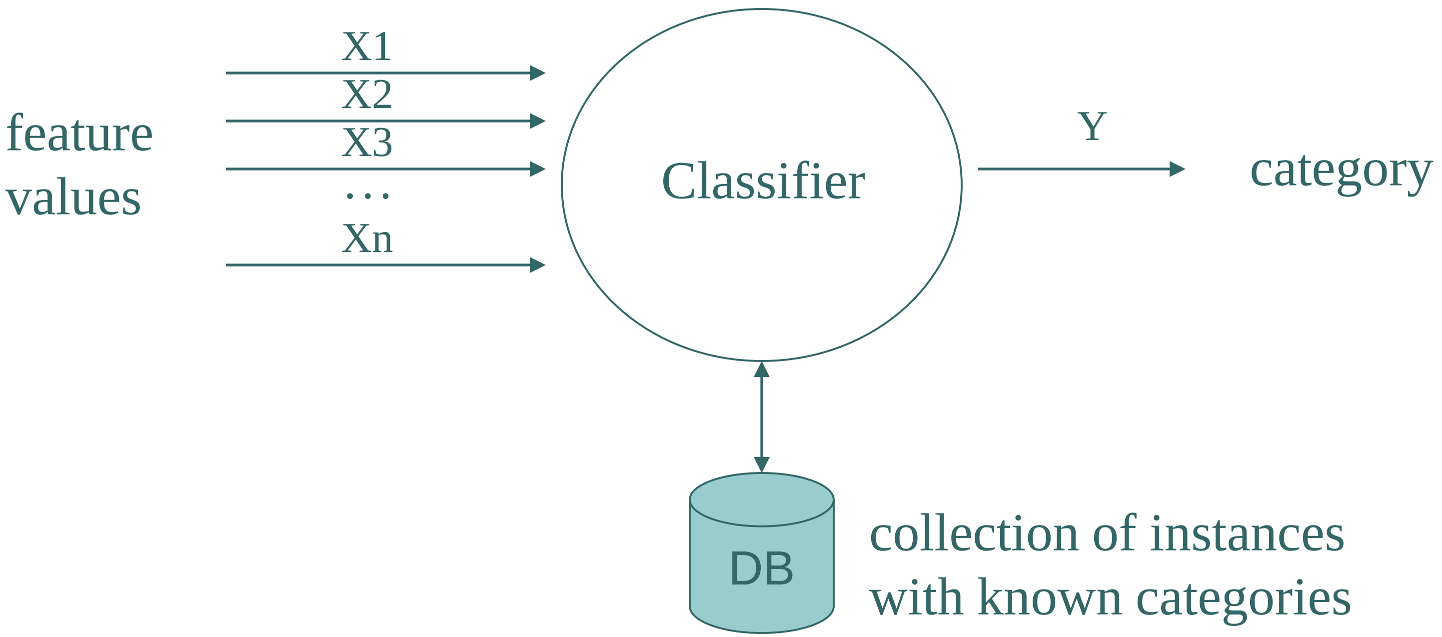
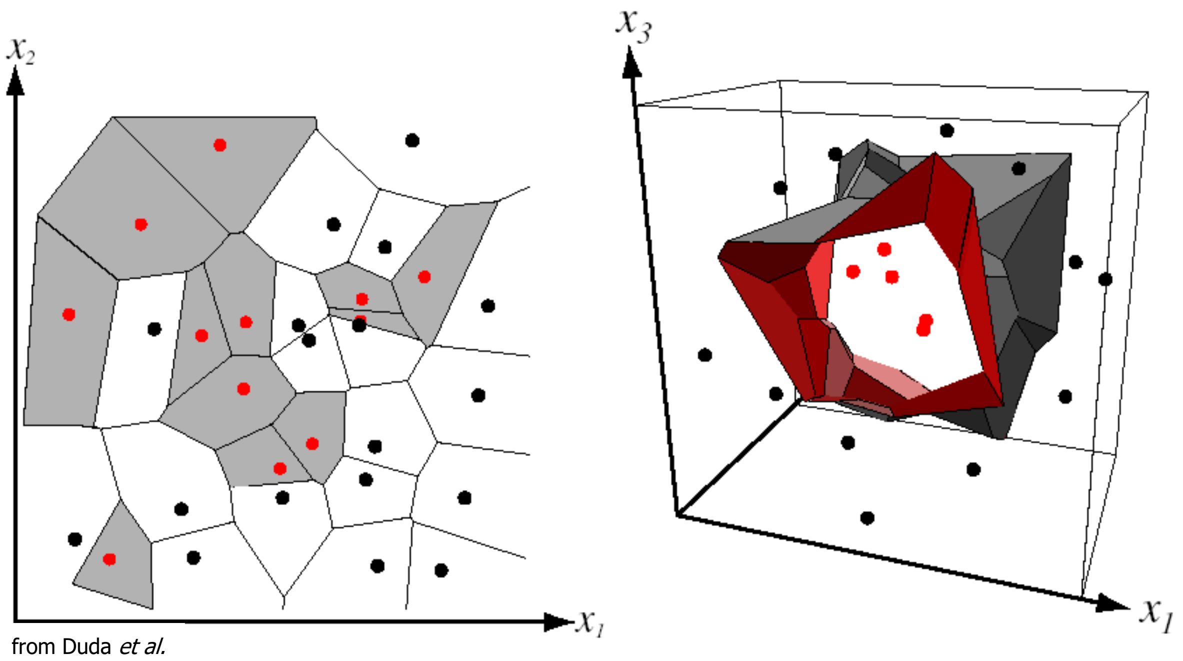
k Nearest Neighbors

Classifiers



Nearest Neighbor Classifier

- Assign label of nearest training data point to each test data point



Voronoi partitioning of feature space
for two-category 2D and 3D data

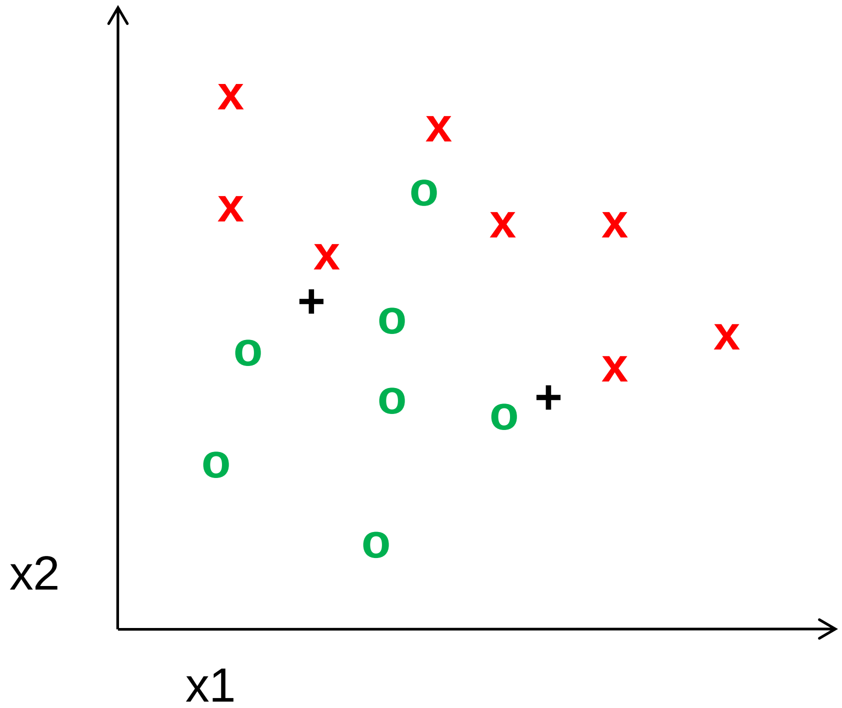
Source: D. Lowe

K - Nearest Neighbors

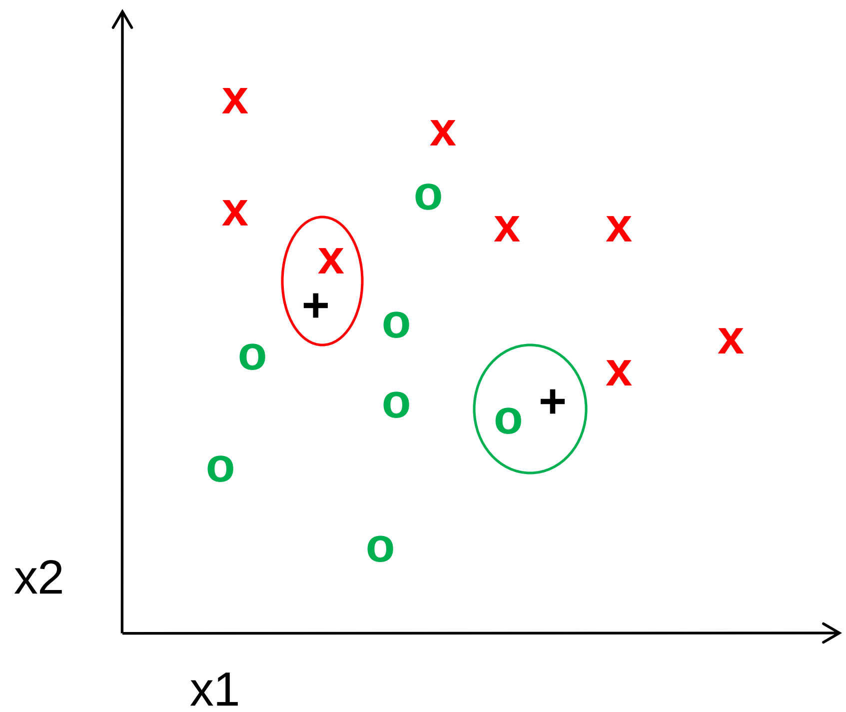
- For a given instance T, get the top k dataset instances that are “nearest” to T
  - Select a reasonable distance measure
- Inspect the category of these k instances, choose the category C that represent the most instances
- Conclude that T belongs to category C

K-nearest neighbor

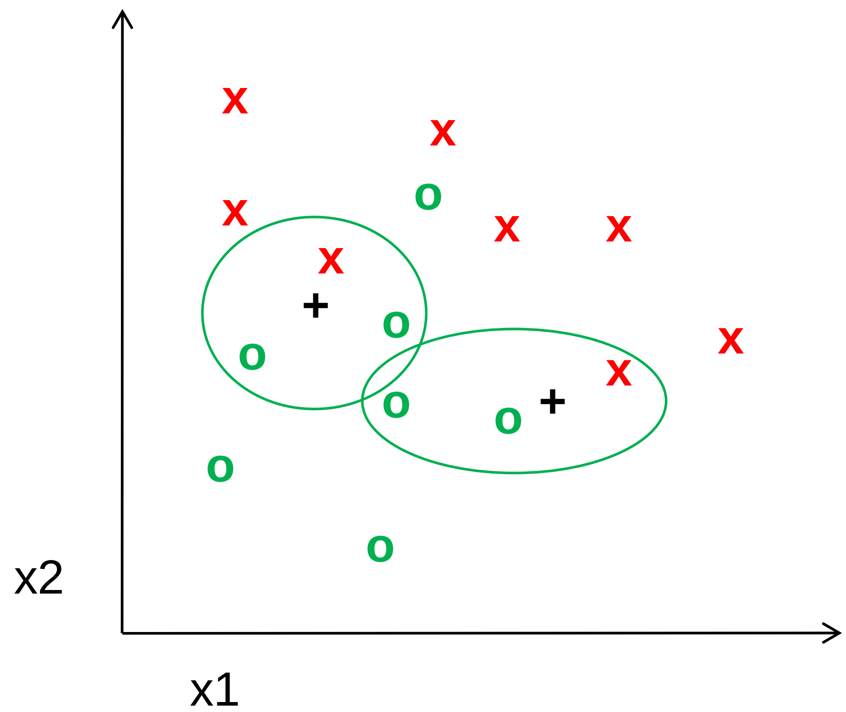
- Let '+' be the new data points, whose class is unknown.



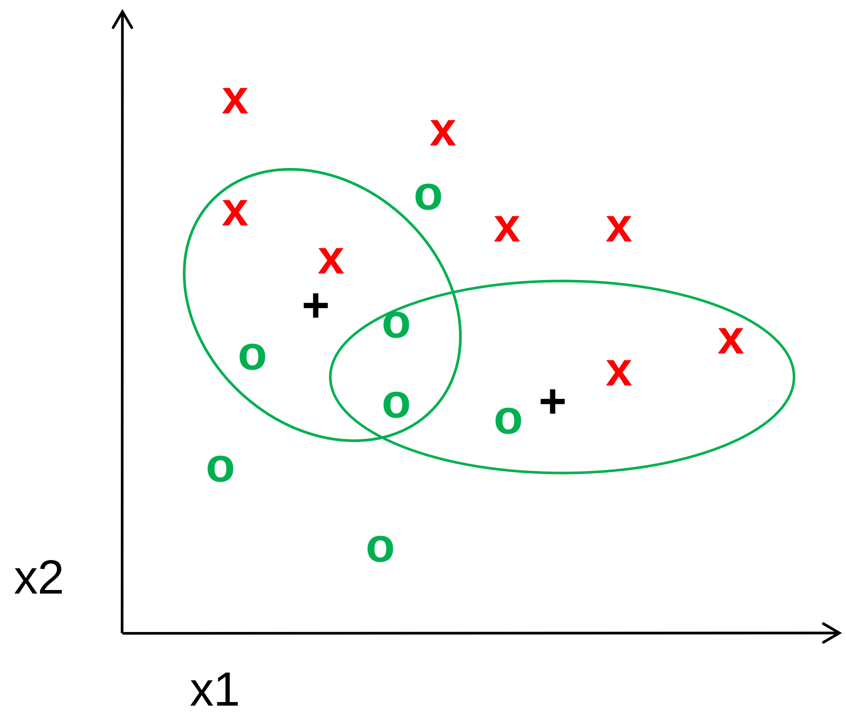
1-nearest neighbor



3-nearest neighbor



5-nearest neighbor



First: Nearest Neighbor (NN) Classifier

- Train
  - Remember all training images and their labels
- Predict
  - Find the closest (most similar) training image
  - Predict its label as the true label

CIFAR-10 and NN results

Example dataset: **CIFAR-10**
10 labels
50,000 training images, each image is tiny: 32x32
10,000 test images.

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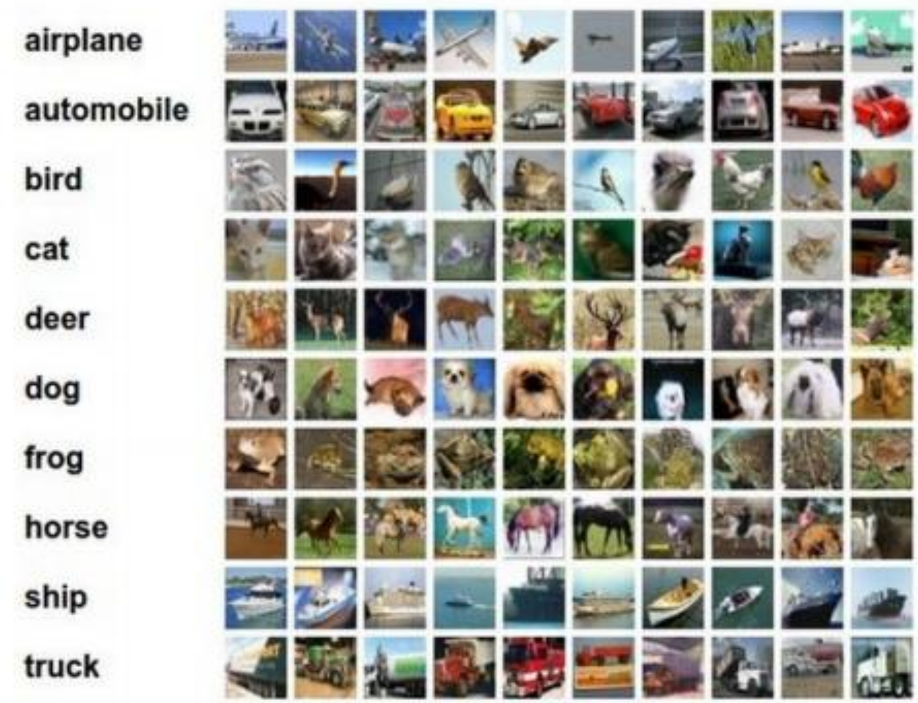
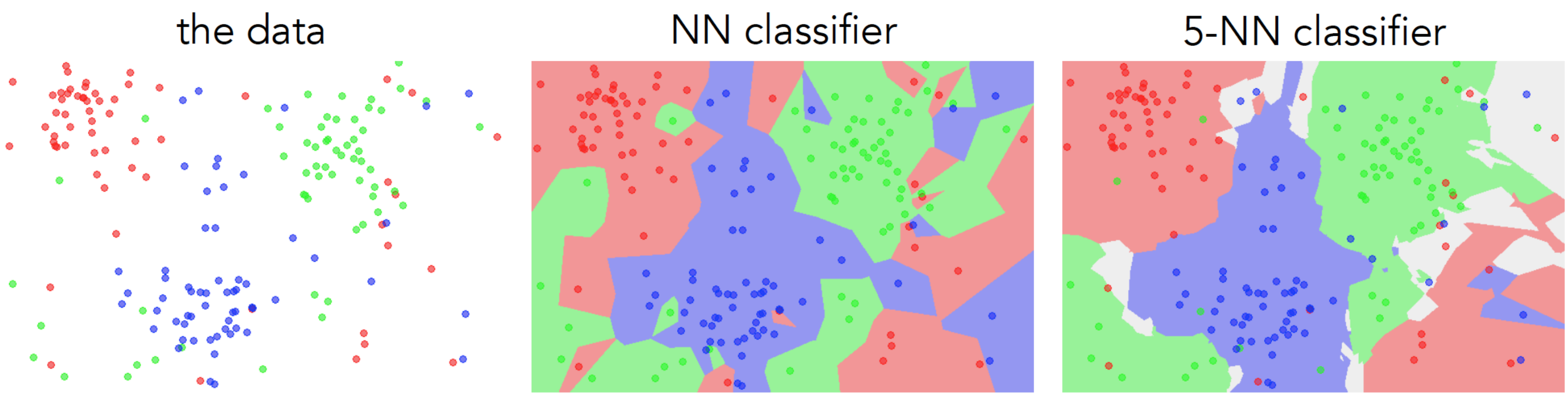


For every test image (first column), examples of nearest neighbors in rows

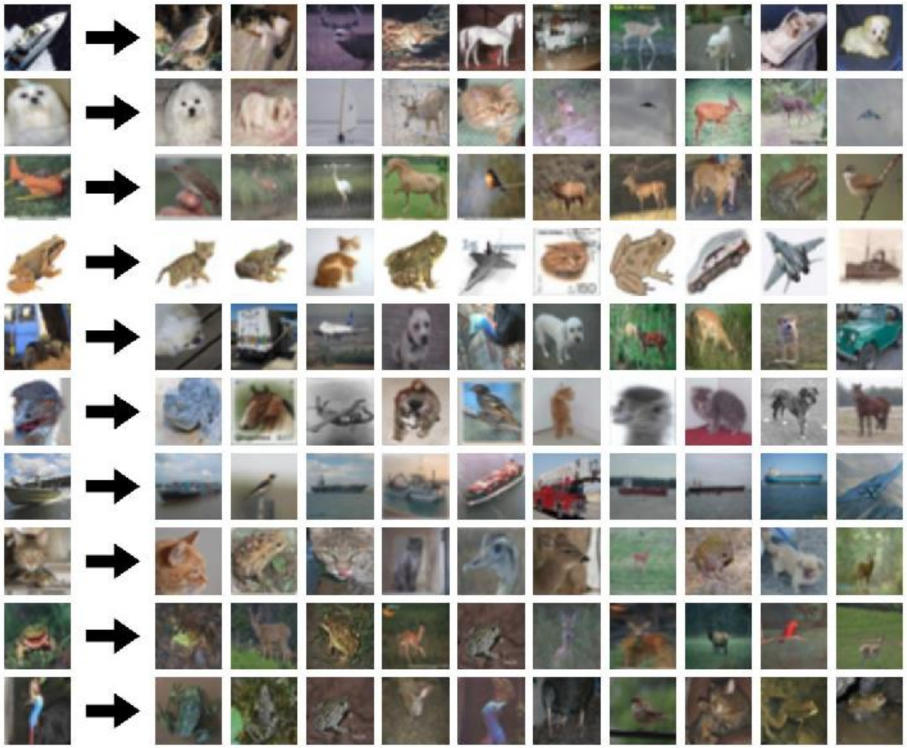
Slides from Andrej Karpathy and Fei-Fei Li
http://vision.stanford.edu/teaching/cs231n/

k-nearest neighbor

- Find the k closest points from training data
- Take **majority vote** from K closest points



What does this look like?



What does this look like?

How to find the most similar training image? What is the distance metric?

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

Where I_1 denotes image 1, and p denotes each pixel

$$\left| \underbrace{\begin{array}{|c|c|c|c|}\hline 56 & 32 & 10 & 18 \\ \hline 90 & 23 & 128 & 133 \\ \hline 24 & 26 & 178 & 200 \\ \hline 2 & 0 & 255 & 220 \\ \hline\end{array}}_{\text{test image}} - \underbrace{\begin{array}{|c|c|c|c|}\hline 10 & 20 & 24 & 17 \\ \hline 8 & 10 & 89 & 100 \\ \hline 12 & 16 & 178 & 170 \\ \hline 4 & 32 & 233 & 112 \\ \hline\end{array}}_{\text{training image}} \right| = \underbrace{\begin{array}{|c|c|c|c|}\hline 46 & 12 & 14 & 1 \\ \hline 82 & 13 & 39 & 33 \\ \hline 12 & 10 & 0 & 30 \\ \hline 2 & 32 & 22 & 108 \\ \hline\end{array}}_{\text{pixel-wise absolute value differences}} \rightarrow 456$$

Slides from Andrej Karpathy and Fei-Fei Li
http://vision.stanford.edu/teaching/cs231n/

Hyperparameters

- What is the **best distance** to use?
- What is the **best value of k** to use?

- These are **hyperparameters**: choices about the algorithm that we set rather than learn

- How do we set them?
  – One option: try them all and see what works best

Choice of distance metric

- Hyperparameter

L1 (Manhattan) distance

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

L2 (Euclidean) distance

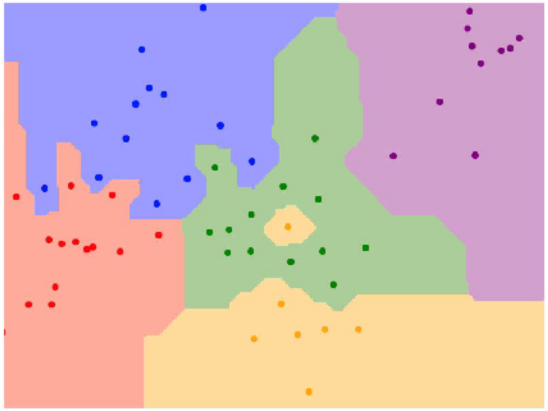
$$d_2(I_1, I_2) = \sqrt{\sum_p \left(I_1^p - I_2^p\right)^2}$$

Slides from Andrej Karpathy and Fei-Fei Li
http://vision.stanford.edu/teaching/cs231n/

K-Nearest Neighbors: Distance Metric

L1 (Manhattan) distance

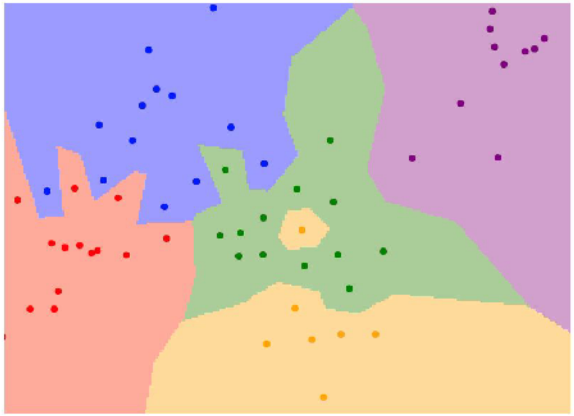
$$d_1(I_1, I_2) = \sum_p |I_1^p - I_2^p|$$



K = 1

L2 (Euclidean) distance

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



K = 1

Demo: http://vision.stanford.edu/teaching/cs231n-demos/knn/

Other distance measures

- City-block distance (Manhattan dist)
  - Add absolute value of differences
- Cosine similarity
  - Measure angle formed by the two samples (with the origin)
- Jaccard distance
  - Determine percentage of exact matches between the samples (not including unavailable data)
- Others

Distance Metrics

Minkowsky:

$$D(\boldsymbol{x},\boldsymbol{y}) = \left(\sum_{i=1}^{m} |x_i - y_i|^r \right)^{1/r}$$

Euclidean:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

Manhattan / city-block:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} |x_i - y_i|$$

Camberra:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{|x_i - y_i|}{|x_i + y_i|}$$

Chebychev:

$$D(\boldsymbol{x},\boldsymbol{y}) = \max_{i=1}^{m} |x_i - y_i|$$

Quadratic:

$$D(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x}-\boldsymbol{y})^T Q (\boldsymbol{x}-\boldsymbol{y}) = \sum_{j=1}^{m} \left(\sum_{i=1}^{m} (x_i - y_i) q_{ji} \right) (x_j - y_j)$$

Q is a problem-specific positive definite $m \times m$ weight matrix

Mahalanobis:

$$D(\boldsymbol{x},\boldsymbol{y}) = [\det V]^{1/m} (\boldsymbol{x}-\boldsymbol{y})^{\mathrm{T}} V^{-1} (\boldsymbol{x}-\boldsymbol{y})$$

V is the covariance matrix of $A_1..A_m$, and A_j is the vector of values for attribute j occuring in the training set instances $1..n$.

Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = \frac{\sum_{i=1}^{m} (x_i - \overline{x_i})(y_i - \overline{y_i})}{\sqrt{\sum_{i=1}^{m} (x_i - \overline{x_i})^2 \sum_{i=1}^{m} (y_i - \overline{y_i})^2}}$$

$\overline{x_i} = \overline{y_i}$ and is the average value for attribute i occuring in the training set.

Chi-square:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{1}{sum_i} \left(\frac{x_i}{size_{\boldsymbol{x}}} - \frac{y_i}{size_{\boldsymbol{y}}} \right)^2$$

sum_i is the sum of all values for attribute i occuring in the training set, and $size_{\boldsymbol{x}}$ is the sum of all values in the vector $\boldsymbol{x}$.

Kendall's Rank Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = 1 - \frac{2}{n(n-1)} \sum_{i=1}^{m} \sum_{j=1}^{i-1} \mathrm{sign}(x_i - x_j)\,\mathrm{sign}(y_i - y_j)$$

sign(x)=-1, 0 or 1 if $x < 0$, $x = 0$, or $x > 0$, respectively.

Figure 1. Equations of selected distance functions.
($\boldsymbol{x}$ and $\boldsymbol{y}$ are vectors of m attribute values).

How to determine the good value for k?

- Determined experimentally
- Start with k=1 and use a test set to validate the error rate of the classifier
- Repeat with k=k+2
- Choose the value of k for which the error rate is minimum

- Note: k should be odd number to avoid ties

Setting Hyperparameters

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

Your Dataset

Setting Hyperparameters

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

BAD: K = 1 always works perfectly on training data

Your Dataset

Setting Hyperparameters

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

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Your Dataset

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

train	test

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

Setting Hyperparameters

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

BAD: K = 1 always works perfectly on training data

Your Dataset

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

train	test

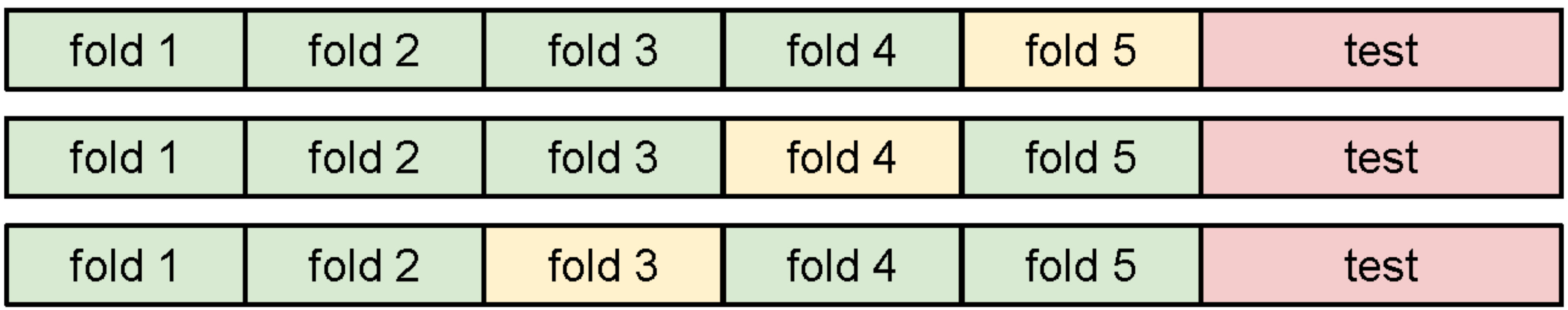
Idea #3: Split data into **train**, **val**, and **test**; choose hyperparameters on val and evaluate on test

Better!

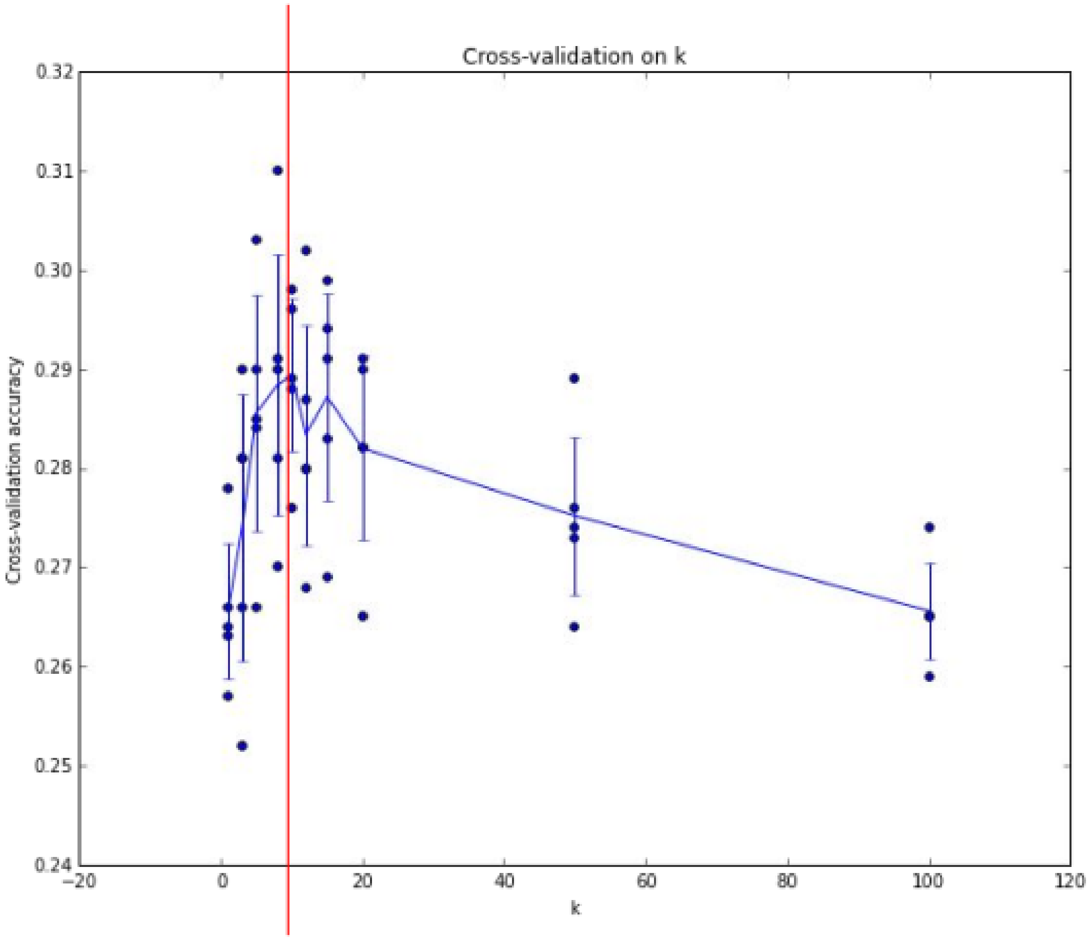
train	validation	test

Setting Hyperparameters

Idea #4: **Cross-Validation**: Split data into **folds**,
try each fold as validation and average the results



Useful for small datasets, but not used too frequently in deep learning



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)

Recap: How to pick hyperparameters?

- Methodology
  - Train and test
  - Train, validate, test

- Train for original model
- Validate to find hyperparameters
- Test to understand generalizability

k-NN Time Complexity

- Suppose there are m instances and n features in the dataset
- Nearest neighbor algorithm requires computing m distances
- Each distance computation involves scanning through each feature value
- Running time complexity is proportional to m X n

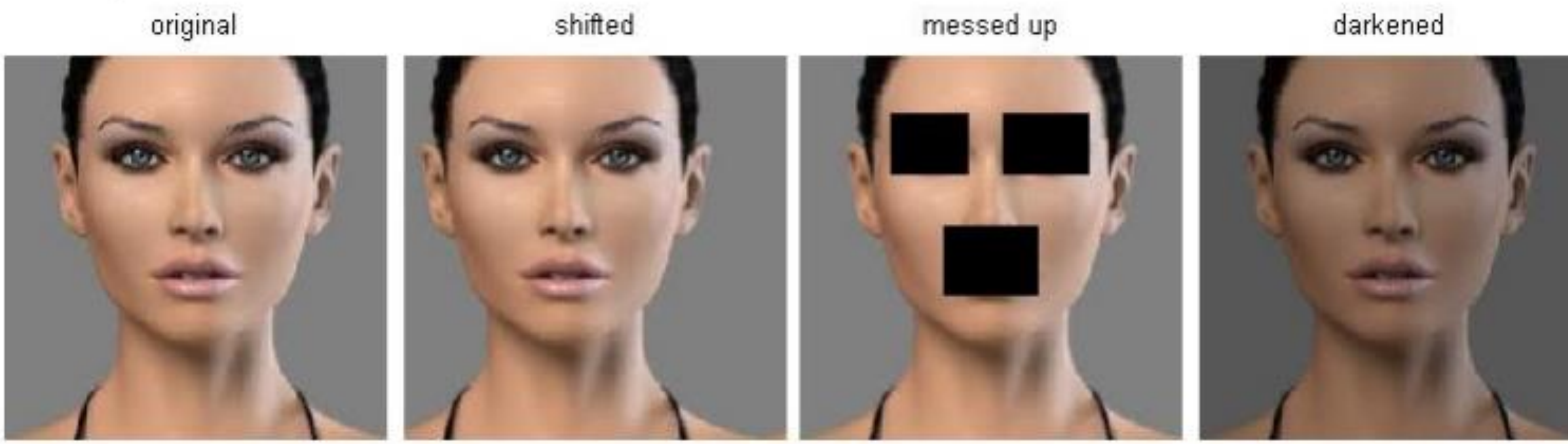
kNN -- Complexity and Storage

- N training images, M test images
- Training: O(1)
- Testing: O(MN)
- Hmm…
  - Normally need the opposite
  - Slow training (ok), fast testing (necessary)

- Disadvantage of kNN (instance-based methods) is that the costs of classifying new instances can be high
- Nearly all computation takes place at classification time rather than learning time

k-Nearest Neighbor on images **never used.**

- terrible performance at test time
- distance metrics on level of whole images can be very unintuitive



(all 3 images have same L2 distance to the one on the left)

k-NN variations

- Value of k
  - Larger k increases confidence in prediction
  - Note that if k is too large, decision may be skewed
- Weighted evaluation of nearest neighbors
  - Plain majority may unfairly skew decision
  - Revise algorithm so that closer neighbors have greater “vote weight”
- Other distance measures

When to Consider Nearest Neighbors

- Instances map to points in R^d
- Less than 20 features (attributes) per instance, typically normalized
- Lots of training data

Advantages:

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

Disadvantages:

- Slow at query time
  - Presorting and indexing training samples into search trees reduces time
- Easily fooled by irrelevant features (attributes)

k-Nearest Neighbors: Summary

- In **image classification** we start with a **training set** of images and labels, and must predict labels on the **test set**
- The **K-Nearest Neighbors** classifier predicts labels based on nearest training examples
- Distance metric and K are **hyperparameters**
- Choose hyperparameters using the **validation set**; only run on the test set once at the very end!