Nearest Neighbour Algorithms

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Outline

Supervised learning

- Given labelled training examples $(x_1, y_1), \dots (x_T, y_T)$ where
- $x_t \in X$ are features
- $y_t \in Y$ are labels..

Feature space $\mathcal{X}$

- Usually $\mathcal{X} = \mathbb{R}^n$: the n-dimensional Euclidean space
- How do we use your class data?

Classification

- $Y = \{1, \dots, m\}$ are discrete labels

Regression

- $Y = \mathbb{R}^m$ are continuous values

The kNN algorithm idea

- Assume an unknown example is similar to its neighbours
- Smoothness allows us to make predictions

Discriminatory analysis-nonparametric discrimination: consistency properties, Evelyn Fix and Joseph L. Hodges Jr, 1951.

Figure: Evelyn Fix

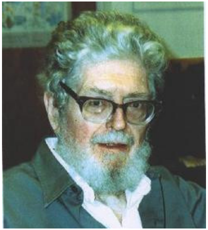
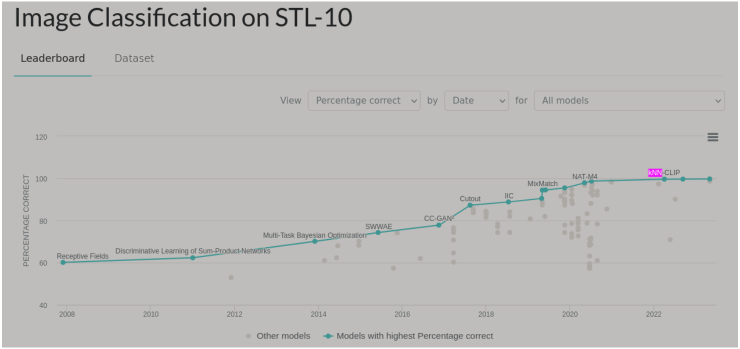


Figure: Joseph Hodges

Performance of KNN on image classification



- Really simple!
- Can outperform really complex models!

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Pseudocode

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$\hat{y}_t \in \mathbb{R}^m$

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- Input: Data $(x_t, y_t)_{t=1}^{T}$, test point x, distance d, neighbours k
- Calculate $h_t = d(x_t, x)$ for all t.
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Classification

- We use a one-hot encoding $(0, \ldots, 0, 1, 0, \ldots, 0)$, with $y_t \in \{0, 1\}^m$.
- The class of the t-th example is $j \Leftrightarrow y_{t,j} = 1$.
- Equivalently, return p with

$$p_i = \sum_{t=1}^{k} \mathbb{I}\left\{y_{s_t} = i\right\}/k$$

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Regression

- $y_t \in \mathbb{R}^m$, so we need do nothing

The number of neighbours

$k = 1$

- How does it perform on the training data?
- How might it perform on unseen data?

$k = T$

- How does it perform on the training data?
- How might it perform on unseen data?

Distance function

For data in $\mathbb{R}^n$, p-norm

$$d(x, y) = \|x - y\|_p$$

Scaled norms

When features having varying scales:

$$d(x, y) = \|Sx - Sy\|_p$$

Or pre-scale the data

Complex data

- Manifold distances
- Graph distance

Distances

A distance $d(\cdot, \cdot)$:

- Identity $d(x, x) = 0$.
- Positivity $d(x, y) > 0$ if $x \neq y$.
- Symmetry $d(y, x) = d(x, y)$.
- Triangle inequality $d(x, y) \leq d(x, z) + d(z, y)$.

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Norms;

A norm $\|\cdot\|$

- Zero element $\|0\| = 0$.
- Homogeneity $\|cx\| = c\|x\|$ for any scalar a.
- Triangle inequality $\|x+y\| \leq \|x\| + \|y\|$.

\$p\$-norm

$$\|z\|_p = \left(\sum_i z_i^p\right)^{1/p}$$

Neighbourhood calculation

If we have T datapoints

Sort and top K.

- Requires $O(T \ln T)$ time

Use the Cover-Tree or KD-Tree algorithm

- Requires $O(cK \ln T)$ time.
- c depends on the data distribution.

Making a decision

kNN as a model

- Given features x, we get a vector p of class probabilities:

$$p_i = P(y = i|x),$$

where $P(y = i|x)$ is the probability that y is i, given x.

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The model versus the prediction

- The model P tells us the probability of different classes.
- When we decide what our prediction should be, we can use the model.
- We will use π to denote the decision rule or policy.

Decisions versus predictions

- We frequently need to make a decision, instead of just a prediction.
- Our utility function $U(y, a)$ represents our preferences.
- The space of actions A is *not identical* to the set of labels Y.

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Minimise spam annoyance

What utility function would you use for the spam detection problem?

Utility	Pass	Flag	Trash
Normal			
Spam			
Virus			

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Classification decision to maximise expected utility

- Expected utility of a single decision

$$\mathbb{E}[U|a, x] = \sum_y P(y|x, a) U(y, a) = \sum_y P(y|x) U(y, a)$$

- The decision maximising expected utility

$$a^* = \arg\max_a \mathbb{E}[U|a, x]$$

KNN activity

- Implement nearest neighbours
- Introduction to scikitlearn nearest neighbours

Homework: Measure performance

In this exercise, you will measure utility on a test set, and select actions that potentially maximise utility in expectation:

Measure utility

Create a function called *utilityScore(y, actions, U)*.
This takes as input the actual labels y_t, and actions a_t (e.g. predicted labels) of a classifier. It then returns the average utility:
$\sum_{t=1}^{T} U(a_t, y_t)/T$.

Calculate utility scores

Calculate the $utility_{score}$ of a basic kNN classifier for various values of k.

Return highest-utility actions

Create a function *predictUtil(clf, X, U)* that takes a classifier *clf*, a dataset of features X and a utility function U as input. It calls $clf.predict\_{proba}()$ and returns a list of actions, one for each row of X.

Verification

Verify that using $\text{predict}_{\text{util}}()$ givs you a higher utilityScore() than simply using predict()