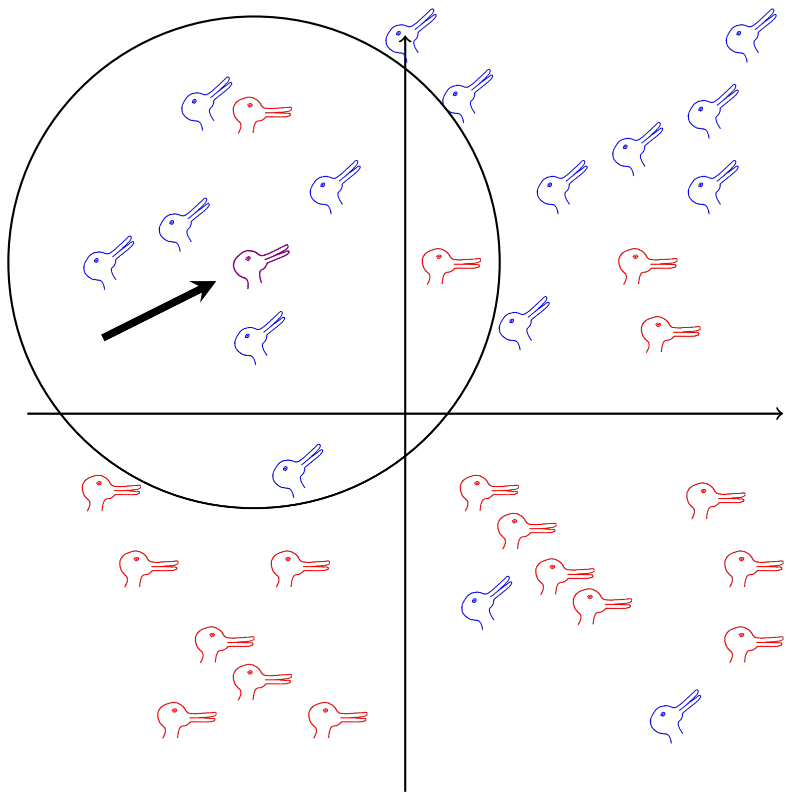
k-Nearest Neighbours.

We will need to think a bit more about the nature of inference, how we can assess it and how we training algorithms, before we do so, it might be useful to look at a couple of examples of supervised learning. We will look at the k-nearest neighbours (k-nn) algorithm first, this algorithm has the virtue of being straight-forward and easy to understand; it is also, in the language of statistical modelling, 'model free', it does not posit a particular structure for the data, though, as we will see, it does assume that the distance measure on the space of data is meaningful. After this we will look at regression, this make a very strong assumption about the structure of the data, but turns out to be both surprisingly useful and an important starting point for thinking about how inference can work. In short, the k-nn algorithm is useful and, perhaps, prompts us to think about 'representations', how we describe the data in numbers, but the following topic, regression, is probably more important as an example of how inference works. Of course, it is good to know about both.

The idea behind k-nn is simple: you have some data $\{(\mathbf{x}_i, y_i)\}$ consisting of input, label pairs. Now, given a new point $\mathbf{x}$ with no label you look at the k nearest points to $\mathbf{x}$ and see what labels they have. You assign $\mathbf{x}$ to whichever label is most common among the neighbours. This raises the question as to what k is, k is what in modern parlance, is called a meta-parameter, it is a number you pick when designing the algorithm; we will discuss the trade-off made in picking k further and, later, we will discuss a procedure for selecting the value.

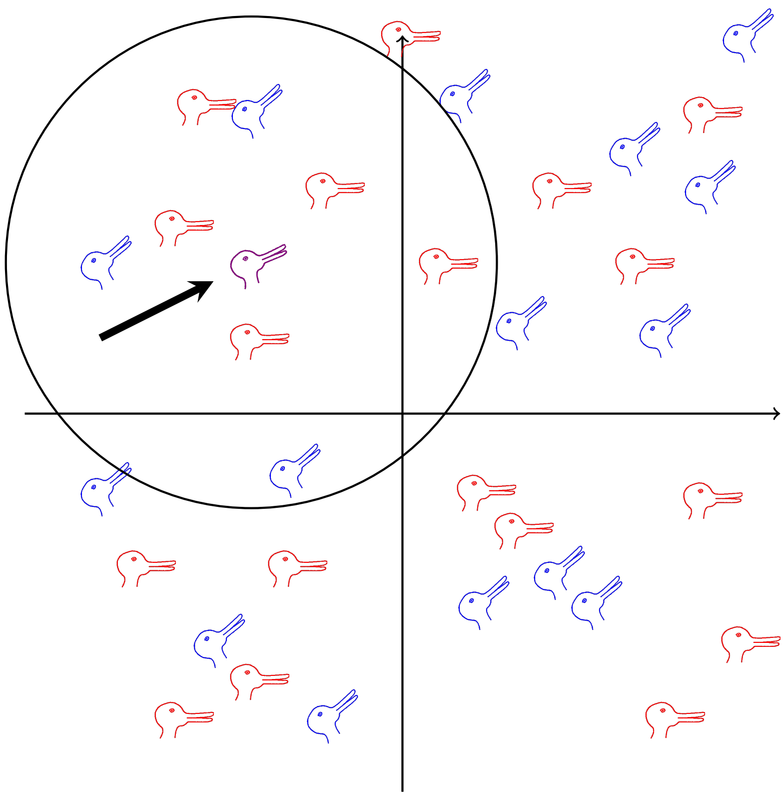
Here is an example; the ducks and rabbits represent the labelled data, the black arrow points towards an unlabelled data point. Here, $k = 8$, the points inside the circle, of these six are rabbits, so the unlabelled point would be labelled a rabbit.



Obviously the notion of k-nearest neighbours relies on a metric on the space the data are in: the obvious thing is to just take the Euclidean distance:

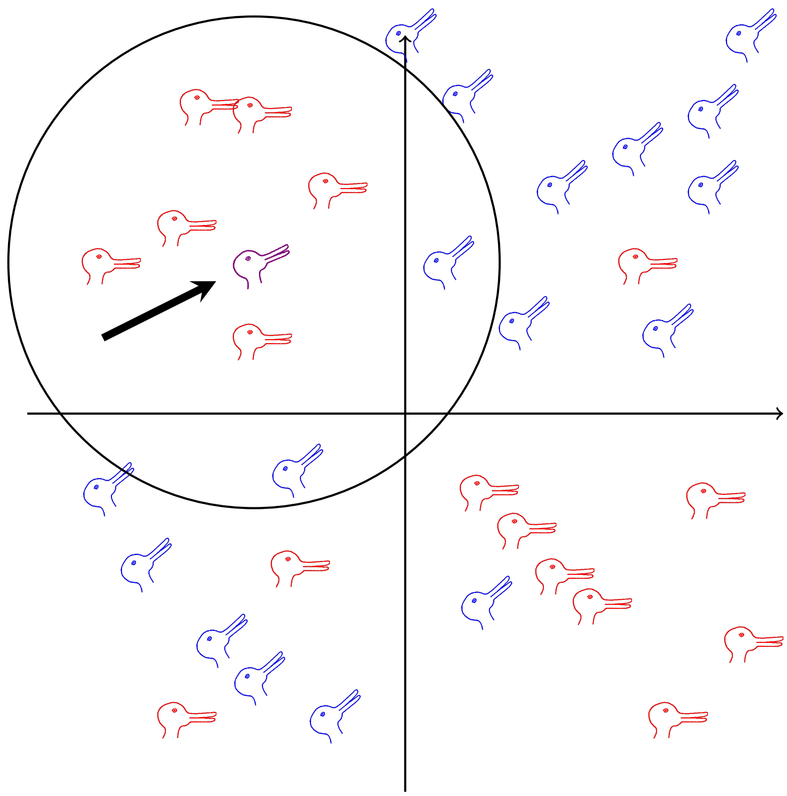
$$\boxed{d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|} \tag{1}$$

but this does reply on the coördinates representing properties of the data relevant to the labelling. If the coördinates have nothing to do with the labelling the approach will not work:



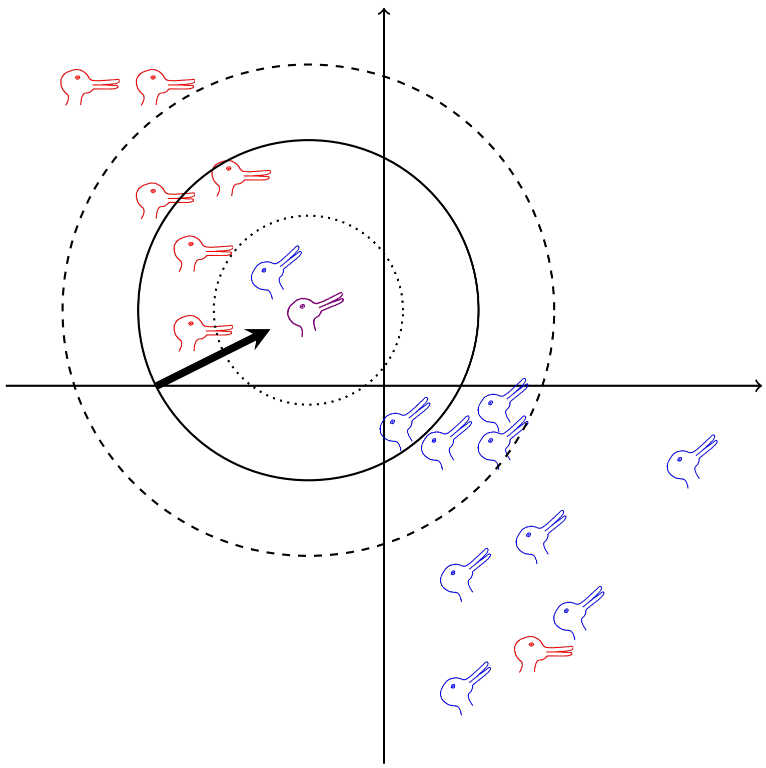
In this case the unlabelled point will be labelled as a duck, but looking at the mix of datapoints it is not clear that that is useful, the location of each point has little to do with its label. This problem is one of representation, the datapoints are being represented by the coördinates, but these may not represent the label in a useful way. In many algorithms some part of the computations relates to finding a good representation, which may involve a mapping of the original coördinate.

Conversely a strength of k-nn is that it does not assume the location represents the label in any particular way, it just assumes that points with a particular label a likely to be near other points with that label, this example shows data where the division between ducks and rabbits does not lie on a single line:



Nonetheless the k-nn approach is useful here. In passing, it should also be noted that the approach does not rely on the distance in a detailed way, it uses it only to calculate proximity. Indeed you might expect the approach to work well even if the space of data does not have coördinates but does have a way of calculating distance, as happens, for example, with time series.

Finally there is the vexing issue of how to pick k. k is a sort of 'smoothing parameter' and as always with smoothing parameters, if it is too small it doesn't smooth and if it is too big it smooths away the stuff you are actually interested in. A very contrived illustration is given here:



Here, it is clear there is a rabbit cluster and a duck cluster; there is a duck in the rabbit cluster and a rabbit in the duck cluster; this represents the possibility of mislabelling or other noise. Now if $k = 5$, corresponding to the cicle with a solid boundary, the unlabelled point is labelled duck, which is probably correct; if $k = 1$ this is a k value much more vulnerable to noise and, indeed here it would result in the unlabelled point being labelled rabbit, similarly, if $k = 9$, corresponding to the dashed circle the neighbourhood is larger than the clustering structure of the label and, again, the unlabelled point would be labelled rabbit.

In the next section we will look at cross-validation, which gives a strategy for picking k.

Summary

In k-nearest neighbours, often called knn or k-nn, you look at the k-nearest points to an unlabelled point and give it the label corresponding to the most common label in the group. It is straight-forward and model free, but does assume the distance you use in ‘nearest’ is meaningful. It also relies on a choice of k, if k is too small then the labelling is vulnerable to noise, if it is too big the labelling might miss the structure of the data.