CS 189 Introduction to Machine Learning
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DIS10

1 Kernelizing Nearest Neighbors

In this question, we will be looking at how we can kernelize k-nearest neighbors (k-NN). k-NN is a simple classifier that relies on nearby training points to decide what a test point's class should be.

Given a test point q, there are two steps to decide what class to predict.

1. Find the k training points nearest q.
2. Return the class with the most votes from the k training points.

For the following parts, assuming that our training points $x \in \mathbb{R}^d$, and that we have n training points.

(a) What is the runtime to classify a newly specified test point q, using the Euclidean distance? (**Hint:** use heaps to keep track of the k smallest distances.)

Solution: To classify a point q, we first need to calculate the distances to every other point. The Euclidean distance is $\sqrt{(x_1 - q_1)^2 + (x_2 - q_2)^2 + \ldots + (x_d - q_d)^2}$, and so for one point, takes $O(d)$ time to compute. For n points, we get $O(nd)$ time.

As we compute the distances, we can use a max-heap to keep track of the k shortest distances seen so far. In the worst case, we have n insertions, taking $O(\log k)$ time each.

This gives us a total run time of $O(nd + n \log k)$.

(b) Let us now "lift" the points into a higher dimensional space by adding all possible mononomials of the original features with degree at most p. What dimension would this space be (asymptotically)? What would the new runtime for classification of a test point q be, in terms of n, d, k, and p?

Solution: Our training points now have d^p features. Therefore, it takes $O(d^p)$ time to compute the Euclidean distance between two points. For n points, the total time is $O(nd^p)$.

We again use a max-heap to keep track of the k shortest distances seen so far. In the worst case, we have n insertions, taking $O(\log k)$ time each.

This gives us a total runtime of $O(nd^p + n \log k)$.

(c) Instead, we can use the polynomial kernel to compute the distance between 2 points in the lifted $O(d^p)$-dimensional space without having to move all of the points into the higher dimensional space. Using the polynomial kernel, $k(x, y) = (x^T y + \alpha)^p$ instead of Euclidean distance, what

is the runtime for k-NN to classify a test point q? (Note: α is a hyperparameter, which can be tuned by validation.)

Solution: Let the $O(d^p)$-dimensional 'lifted' point corresponding to a point x in d-dimensional space be represented by $\Phi(x)$. The Euclidean distance squared between the test point q and a training point x in the 'lifted' space is $\|\Phi(q) - \Phi(x)\|^2$. We then have:

$$\begin{aligned}\|\Phi(q) - \Phi(x)\|^2 &= \Phi^T(q)\Phi(q) - 2\Phi^T(q)\Phi(x) + \Phi^T(x)\Phi(x) \\ &= k(q,q) - 2k(q,x) + k(x,x)\end{aligned}$$

We note that the kernel calculations take $O(d)$ time. Therefore, for n points, we get $O(nd)$ time. Following the same logic as before, we end up with a total runtime of $0(nd + n \log k)$.

Note: We assume that exponentiation (a^b) of two floating-point numbers a, b takes $O(1)$ time.

2 When is $k(x, y)$ a Kernel?

Let $\mathbb{R}^d$ be the vector space that contains our training and test points. For a function $k : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ to be a valid kernel, it suffices to show that either of the following conditions is true:

1. k has an inner product representation: $\exists\ \Phi : \mathbb{R}^d \to \mathcal{H}$, where $\mathcal{H}$ is some (possibly infinite-dimensional) inner product space such that $\forall x_i, x_j \in \mathbb{R}^d,\ k(x_i, x_j) = \Phi^T(x_i)\Phi(x_j)$.
2. For every sample $x_1, x_2, \ldots, x_n \in R^d$, the kernel matrix

$$K = \begin{bmatrix} k(x_1,x_1) & \cdots & k(x_1,x_n) \\ \vdots & k(x_i,x_j) & \vdots \\ k(x_n,x_1) & \cdots & k(x_n,x_n) \end{bmatrix}$$

   is positive semidefinite.

(a) Show that the first condition implies the second one, i.e. if $\forall x_i, x_j \in \mathbb{R}^d,\ k(x_i, x_j) = \Phi^T(x_i)\Phi(x_j)$ then the kernel matrix K is PSD.

Solution: $\forall a \in \mathbb{R}^n, a^T K a = \sum_{i,j} a_i a_j k(x_i, x_j) = \sum_{i,j} a_i a_j \Phi^T(x_i)\Phi(x_j) = \|\sum_i a_i \Phi(x_i)\|_2^2 \geq 0$

(b) Given a positive semidefinite matrix A, show that $k(x_i, x_j) = x_i^\top A x_j$ is a valid kernel.

Solution: We can show k admits a valid inner product representation:

$$k(x_i, x_j) = x_i^\top A x_j = x_i^\top P D^{1/2} D^{1/2} P^\top x_j = \langle D^{1/2} P^\top x_i, D^{1/2} P^\top x_j \rangle = \langle \Phi(x_i), \Phi(x_j) \rangle$$

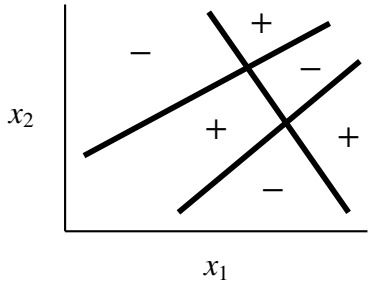
where $\Phi(x) = D^{1/2} P^\top x$

(c) Show why $k(x_i, x_j) = x_i^\top(\text{rev}(x_j))$ (where rev(x) reverses the order of the components in x) is *not* a valid kernel.

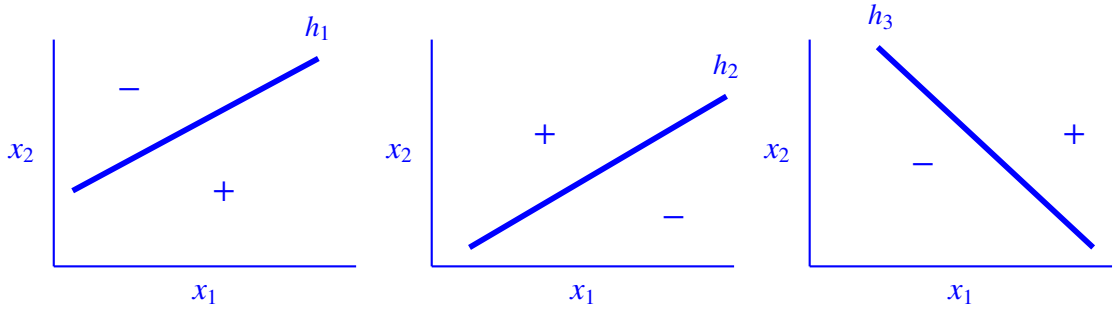
Solution: A counterexample: We have that $k((-1,1),(-1,1)) = -2$, but this is invalid since if k is a valid kernel then $\forall x,\ k(x,x) = \langle \Phi(x), \Phi(x) \rangle \geq 0$.

3 The Multi-layer Perceptron (MLP)

(a) Consider a target function whose + and − regions are illustrated below. Draw the perceptron components, and express f as a Boolean function of its perceptron components.



Solution: The perceptrons correspond to the three lines in the target function. The choice of signs for each one is a bit arbitrary, but ours makes the notation in the next part convenient.



To form the Boolean function, we focus on when f is +. The top + region contributes $\bar{h}_1 h_2 h_3$ to f. The lower left + region contributes $h_1 h_2 \bar{h}_3$ to f. The lower right + region contributes $h_1 \bar{h}_2 h_3$ to f. Combining these, we have: $f = \bar{h}_1 h_2 h_3 + h_1 h_2 \bar{h}_3 + h_1 \bar{h}_2 h_3$.

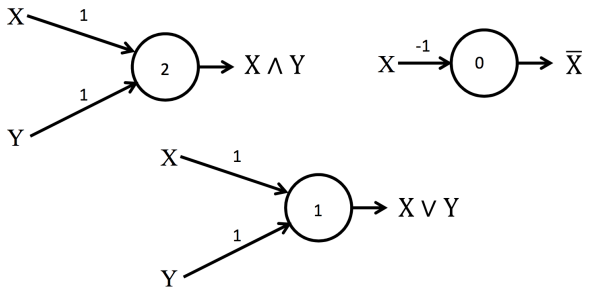
Take-away: a complicated target function, such as the one above, that is composed of perceptrons can be expressed as an `OR` of `AND`s of the component perceptrons.

Let's develop some intuition for why this might be useful.

(b) Over two inputs x_1 and x_2, how can `OR`, `AND`, and `NOT` each be implemented by a single perceptron? What about `NAND` and `NOR`? Assume each unit uses a *hard threshold* activation function: for a constant α,

$$h(x) = \begin{cases} 1 & \text{if } w^\top x \geq \alpha, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

Solution:



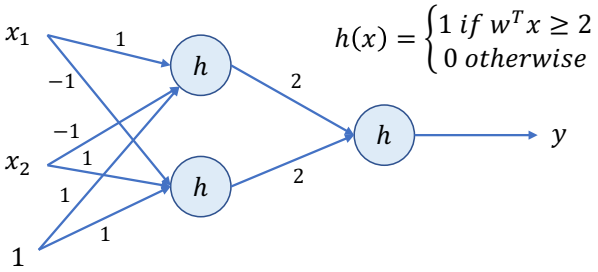
(c) For any Boolean function f, can we build a neural network with at most one hidden layer to compute f?

Solution: We can prove this by construction. Any Boolean function can be represented using a combination of `NOT`, `AND`, `OR` gates. Each of these gates is easily represented by a neural network. We don't provide a formal proof of this statement, but instead provide an example to motivate your intuition.

Consider the boolean function from part (a), which was $f(x_1, x_2, x_3) = \bar{x}_1 x_2 x_3 + x_1 x_2 \bar{x}_3 + x_1 \bar{x}_2 x_3$. This can be expressed as a 3-input network with 3 nodes in a hidden layer that goes to a summation node with scalar output. Each node in the hidden layer computes one of the expressions in the sum.

(d) We have seen that `XOR` is not linearly separable, and hence it cannot be implemented by a single perceptron. Draw a fully connected three-unit neural network that has binary inputs $X_1, X_2, \mathbf{1}$ and output Y, where Y implements the `XOR` function $Y = \texttt{XOR}(X_1, X_2)$. Again, assume each unit uses a *hard threshold* activation function.

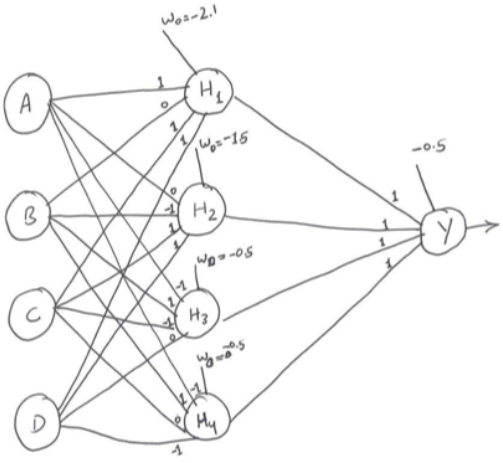
Solution:



(e) (self-study) Create a neural network with a single hidden layer (of any number of units) that implements the function (A or NOT B) XOR (NOT C or NOT D).

Solution: `XOR` can be expressed in terms of `AND` and `OR` functions: p `XOR` $q = (p\bar{q}) + (\bar{p}q)$. Therefore, we can re-write the original expression as: ((A or not B) and not (not C or not D)) or (not (A or not B) and (not C or not D)). Simplifying gives: (A and C and D) or (not B and C and D) or (not A and B and not C) or (not A and B and not D).

We can represent this with 4 inputs (A,B,C,D), and 4 hidden nodes in one hidden layer that feed into the summation node that gives the output. Each hidden node corresponds to one `AND` expression (i.e., one expression in parentheses) in the simplified expression of `OR`s above. One possible network that implements this is:



Take-away: If f can be decomposed into perceptrons using an `OR` (or `NOR`) of `AND`s, then it can be implemented by a 3-layer perceptron. A one-hidden-layer MLP is a universal Boolean function. How cool is that?!

Solution: Very cool!! Though in practice though this is not particularly useful, as it can require an exponentially large number of perceptrons.

4 Mercer's Theorem (Optional)

A vast variety of algorithms in Machine Learning involve calculating dot products of d-dimensional feature vectors. These algorithms can be strengthened by adding nonlinear combinations of the original features as new features. However, calculating the dot products of the new, larger, feature vectors can take much longer. The 'kernel trick' solves this very elegantly by expressing the dot products of the longer vectors as functions of vectors in the original d-dimensional space.

We saw in class that the quadratic kernel could be written as the dot product of two higher dimensional vectors (considering only two features for simplicity):

$$\begin{aligned}(x^T z + 1)^2 &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2 + 2x_1 z_1 + 2x_2 z_2 + 1 \\ &= \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1 x_2 & \sqrt{2}x_1 & \sqrt{2}x_2 & 1 \end{bmatrix} \cdot \begin{bmatrix} z_1^2 & z_2^2 & \sqrt{2}z_1 z_2 & \sqrt{2}z_1 & \sqrt{2}z_2 & 1 \end{bmatrix}^T \\ &= \Phi^T(x)\Phi(z)\end{aligned}$$

In this problem, we shall learn how to decompose a general kernel function $k : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ into a dot product of two higher-dimensional vectors. For technical purposes, we shall assume that $k(x, y)$ satisfies the Hilbert-Schmidt condition, $\int k^2(x, y)\, dxdy < \infty$. We shall first define a vector space F consisting of (so-called L^2) functions $f : \mathbb{R}^d \mapsto \mathbb{R}$.

Recall that a linear transformation from a vector r to a vector s can be written using a matrix A as $s(i) = \sum_j A(i, j)r(j)$.

(a) Write down the linear transformation L_k from function space to function space, $L_k : F \mapsto F$, that the kernel function $k(x, y)$ induces.

Solution: Let us denote by $L_k(f)$ the result of applying the linear transformation on f. Then, we have:

$$L_k(f)(x) = \int_{y \in \mathbb{R}^d} k(x, y) f(y)\, dy$$

(b) How would one define eigenfunctions $\phi(x)$ of L_k?

Solution: Eigenfunctions of L_k are those that satisfy:

$$\int_{y \in \mathbb{R}^d} k(x, y) \phi(y)\, dy = \lambda_\phi \phi(x)$$

Since the kernel function is symmetric positive semi definite, it is possible to prove that the above eigenvalues are all non-negative and that the eigenfunctions are orthonormal. This statement is called Mercer's Theorem. Recall that the eigendecomposition for symmetric A can be written (component-wise) as $A(i, j) = \sum_k \lambda_k v_k(i) v_k(j)$.

(c) In analogy with the eigendecomposition for matrices, write down the eigendecomposition for the kernel function $k(x, y)$ in terms of its eigenvalues and eigenvectors. Then, write it as a dot product of two higher-dimensional (possibly infinite dimensional) vectors $\Phi(x)$ and $\Phi(y)$.

Solution: Let the rank of the linear transformation induced by k be r. For kernels such as rbf, r is infinite.

$$\begin{aligned} k(x, y) &= \sum_{i=1}^{r} \lambda_{\phi_i} \phi_i(x) \phi_i(y) \\ &= \left[\sqrt{\lambda_{\phi_i}} \phi_i(x) \right]_{i=1}^{r} \cdot \left[\sqrt{\lambda_{\phi_i}} \phi_i(y) \right]_{i=1}^{r} \\ &= \Phi^T(x) \Phi(y) \end{aligned}$$

Therefore, the higher-dimensional 'lifted' form of vector x is given by the vector $\Phi(x) = \left[\sqrt{\lambda_{\phi_i}} \phi_i(x) \right]_{i=1}^{r}$.

The takeaway from this problem is that the features of the higher-dimensional vectors that get created by the use of a kernel function are precisely the eigenfunctions of the kernel multiplied by the square-root of their respective eigenvalues.