Introduction to Machine Learning, Fall 2015 - Exercise session V

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Problem 2 (3 points)

Exclusive or is a classical example used to demonstrate the limitations of linear classifiers. In the most basic setting, we have two binary inputs and a binary output. Using +1 and -1 as the binary values, the exclusive or function XOR is given by the following table:

x_1	x_2	$\text{XOR}(x_1, x_2)$
-1	-1	-1
-1	+1	+1
+1	-1	+1
+1	+1	-1

(a) Give a detailed proof for the fact that the exclusive or function cannot be represented as a linear classifier. That is, prove that there is no coefficient vector (w_0, w_1, w_2) such that

$$\text{XOR}(x_1, x_2) = \text{sign}(w_0 + w_1 x_1 + w_2 + x_2)$$

whould hold for all possible inputs (x_1, x_2).

(b) Show that if we include an extra input variable $x_1 x_2$, we can represent XOR as a linear classifier in terms of the modified inputs. That is, find a coefficient vector (w_0, w_1, w_2, w_3) such that

$$\text{XOR}(x_1, x_2) = sign(w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2)$$

holds for all (x_1, x_2).

Solution to (a)

Define three points in $\mathbb{R}^3$:

A $(-1, -1, w_0 - w_1 - w_2)$,

B $(-1, +1, w_0 - w_1 + w_2)$,

C $(+1, -1, w_0 + w_1 - w_2)$.

We must have

$$\begin{aligned} w_0 - w_1 - w_2 &< 0, \\ w_0 - w_1 + w_2 &> 0, \\ w_0 + w_1 - w_2 &> 0. \end{aligned}$$

Next, let us find a plane in $\mathbb{R}^3$ that passes through points A, B and C: $z = ax + by + c$. Now,

$$\begin{cases} -a - b + c & = w_0 - w_1 - w_2 \\ -a + b + c & = w_0 - w_1 + w_2 \\ a - b + c & = w_0 + w_1 - w_2, \end{cases}$$

which simplifies to

$$\begin{cases} -a - b + c & = w_0 - w_1 - w_2 \\ 2c & = 2w_0, \end{cases}$$

so we have that $c = w_0$. Next,

$$\begin{cases} -a - b & = -w_1 - w_2 \\ -a + b & = -w_1 + w_2. \end{cases}$$

Which leads to $-2a = -2w_1$ and $a = w_1$, and finally $b = w_2$. Now our plane is defined as

$$z = w_1 x + w_2 y + w_0.$$

The point D has coordinates $(+1, +1, w_0 + w_1 + w_2)$. Since

$$\begin{aligned} w_0 - w_1 + w_2 &> 0 \\ w_0 + w_1 - w_2 &> 0, \end{aligned}$$

summing the above inequalities we obtain $w_0 > 0$. Also, since $w_0 - w_1 - w_2 < 0$, we have that $w_0 < w_1 + w_2$. So $w_0 + w_1 + w_2 > 0$ and D is “misclassified” (we should have had $w_0 + w_1 + w_2 < 0$.).

If we chose instead of the point D another point, we would get the same contradiction. The problem is that all four points do not lie on a same single plane, and this model is linear, which implies that there is no such “desicion plane” that could handle all four cases.

Solution to (b)

This one is easy. Just define $\text{XOR}(x_1, x_2) = -\text{sign}(x_1 x_2)$. Now

x_1	x_2	XOR(x_1, x_2)
-1	-1	$-\text{sign}((-1) \times (-1)) = -\text{sign}(1) = -1$
-1	+1	$-\text{sign}((-1) \times (+1)) = -\text{sign}(-1) = 1$
+1	-1	$-\text{sign}((+1) \times (-1)) = -\text{sign}(-1) = 1$
+1	+1	$-\text{sign}((+1) \times (+1)) = -\text{sign}(1) = -1$

Problem 3 (3 points)

Multilayer neural networks are another way of using linear classifiers for non-linear problems. The most basic such classifier, for two-dimensional inputs and with two *hidden units*, has parameters (u_{ij}), $i \in \{1, 2\}$, $j \in \{0, 1, 2\}$ and (v_k), $i \in \{0, 1, 2\}$ (that is, a total of 9 parameters), and computes a mapping $(x_1, x_2) \mapsto y$ as follows:

$$
\begin{aligned}
z_1 &= \text{sign}(u_{10} + u_{11}x_1 + u_{12}x_2) \\
z_2 &= \text{sign}(u_{20} + u_{21}x_1 + u_{22}x_2) \\
7 &= \text{sign}(v_0 + v_1 z_1 + v_2 z_2).
\end{aligned}
$$

[The figure omitted.] The term "hidden unit" refers to the computation of intermediate values z_i that are not as such part of the visible input or output.

(a) Show that with a suitable choice of the weights (u_{ij}) and (v_k), the neural network explained aboce can compute the XOR function from Problem 2.

(b) There are numerous variants of this basic neural network model. In particular, the signum function used above in computing the values z_i is often replaced by some continuous function, such as the logistic sigmoid $r \mapsto 1/(1 + e^{-r})$. However, one variant that does *not* make sense is just to ignore the signum function for z_i and just compute

$$
\begin{aligned}
z_1 &= u_{10} + u_{11}x_1 + u_{12}x_2 \\
z_2 &= u_{20} + u_{21}x_1 + u_{22}x_2 \\
y &= \text{sign}(v_0 + v_1 z_1 + v_2 z_2).
\end{aligned}
$$

Show that this model would not offer any advantage over a basic linear classifier $y = \text{sign}(w_0 + w_1 x_1 + w_2 x_2)$.

Solution to (a)

If we restrict the values of $v_0, v_1, v_2, u_{10}, u_{11}, u_{12}, u_{20}, u_{21}, u_{22}$ to the set $\{-1, +1\}$, there is 16 possible assignments such that the neural network in question computes XOR(x_1, x_2). One of them is

$$\begin{aligned} v_0 &= -1 \\ v_1 &= +1 \\ v_2 &= -1 \\ u_{10} &= +1 \\ u_{11} &= -1 \\ u_{12} &= -1 \\ u_{20} &= -1 \\ u_{21} &= -1 \\ u_{22} &= -1 \end{aligned}$$

x_1	x_2	z_1	z_2	y
-1	-1	+1	+1	-1
-1	+1	+1	-1	+1
+1	-1	+1	-1	+1
+1	+1	-1	-1	-1

Solution to (b)

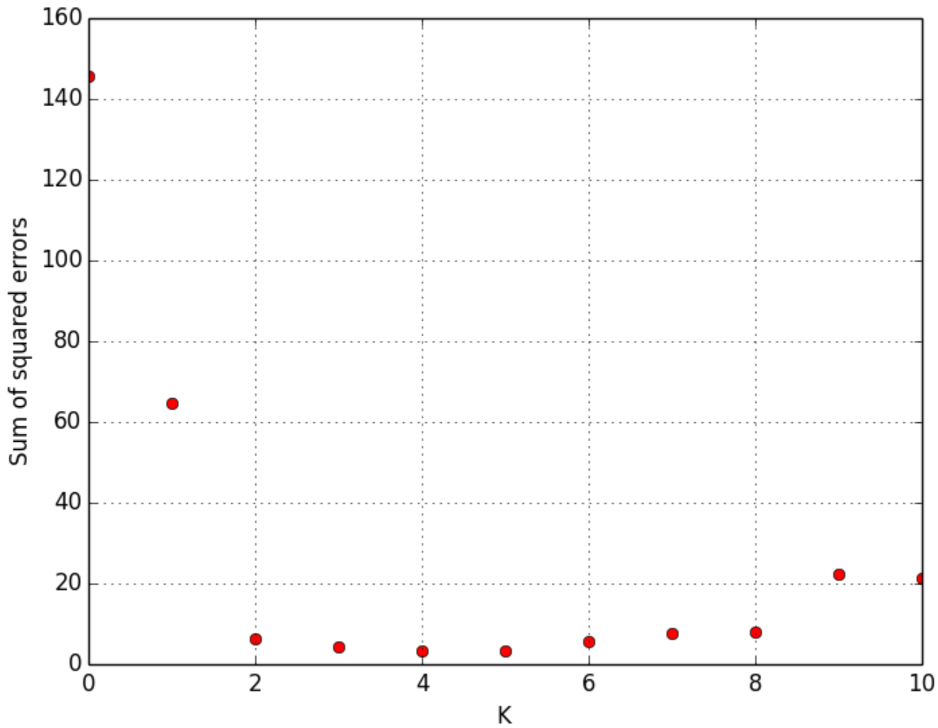
We have that

$$\begin{aligned} y &= \operatorname{sign}(v_0 + v_1 z_1 + v_2 z_2) \\ &= \operatorname{sign}(v_0 + v_1(u_{10} + u_{11}x_1 + u_{12}x_2) + v_2(u_{20} + u_{21}x_1 + u_{22}x_2)) \\ &= \operatorname{sign}(\overbrace{(v_0 + v_1 u_{10} + v_2 u_{20})}^{w_0} + \overbrace{(v_1 u_{11} + v_2 u_{21})}^{w_1} x_1 + \overbrace{(v_1 u_{12} + v_2 u_{22})}^{w_2} x_2), \end{aligned}$$

which is exactly what we had in Problem 2 (a).

4 (15 points)

What comes to the (a) part, just run the Python script (013593012.py) and it will show the fitting polynomials for $K = 0, 1, \ldots, 10$. The figure I got is:



It would seem that $K = 4$ would work best, but the best K varies from time to time. After $K = 5$, the error does not really improve and becomes large at $K = 9$. On another run of the program, I got that $K = 3$ is the best with sum of squared errors of ~ 4.9 and coefficients something like

$$(\overbrace{0.006}^{x^3}, \overbrace{-0.520}^{x^2}, \overbrace{0.994}^{x}, 2.019),$$

which is almost the target polynomial with minor "corrections". (**Note**: I have excluded the printing of the actual coefficients for the task (b), as there is too much of it.)