Machine Learning: Homework #6

Due on Monday, November 6, 2017 $Abu\text{-}Mostafa\ 3:00pm$

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Overfitting and Deterministic Noise

Problem 1

Deterministic noise depends on \mathcal{H} , as some models approximate f better than others. Assume that $\mathcal{H}' \subset \mathcal{H}$ and that f is fixed. In general (but not necessarily in all cases), if we use \mathcal{H}' instead of \mathcal{H} , how does deterministic noise behave?

- (a) In general, deterministic noise will decrease.
- (b) In general, deterministic noise will increase.
- (c) In general, deterministic noise will be the same.
- (d) There is deterministic noise for only one of \mathcal{H} and \mathcal{H}' .

Let $(h')^*(x) \in \mathcal{H}'$ be the best possible approximation of f(x) in \mathcal{H}' , that is $\|(f - (h')^*)(x)\|$ is as small as possible. However because $\mathcal{H}' \subset \mathcal{H}$, then $(h')^* \in \mathcal{H}$ and if we define h'(x) to be the best possible approximation of f in \mathcal{H} , then $\|(h' - f)(x)\| \leq \|((h')^* - f)(x)\|$. Therefore, in general deterministic noise will monotonically increase if we use \mathcal{H}' .

Regularization with Weight Decay

In the following problems use the data provided in the files

http://work.caltech.edu/data/in.dta http://work.caltech.edu/data/out.dta

as a training and test set respectively. Each line of the files corresponds to a two-dimensional input $\mathbf{x} = (x_1, x_2)$, so that $\mathcal{X} = \mathbb{R}^2$, followed by the corresponding label from $\mathcal{Y} = \{-1, 1\}$. We are going to apply Linear Regression with a non-linear transformation for classification. The nonlinear transformation is given by

$$\Phi(x_1, x_2) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2, |x_1 - x_2|, |x_1 + x_2|).$$

Recall that the classification error is defined as the fraction of misclassified points.

Problem 2

Run Linear Regression on the training set after performing the non-linear transformation. What values are closest (in Euclidean distance) to the in-sample and out-of-sample classification errors, respectively?

- (a) 0.03, 0.08
- (b) 0.03, 0.10
- (c) 0.04, 0.09
- (d) 0.04, 0.11
- (e) 0.05, 0.10

For details, see the Jupyter notebook containing the code for this section. Below are the in-sample and out-of-sample errors for several different choices of the weight decay parameter $\lambda = 10^k$.

```
Without regularization
E_{in} = 0.029 E_{out} = 0.084
With regularization parameter k = -3
E_{in} = 0.029 E_{out} = 0.080
With regularization parameter k = -2
E_{in} = 0.029 E_{out} = 0.084
With regularization parameter k = -1
E_{in} = 0.029 E_{out} = 0.056
With regularization parameter k = 0
E_{in} = 0.000 E_{out} = 0.092
With regularization parameter k = 1
E_{in} = 0.057 E_{out} = 0.124
With regularization parameter k = 2
E_{in} = 0.200 E_{out} = 0.228
With regularization parameter k = 3
E_{in} = 0.371 E_{out} = 0.436
```

Problem 3

Now add weight decay to Linear Reression , that is, add the term $\frac{\lambda}{N}\sum_{i=0}^{7}w_{i}^{2}$ to the squared in-sample error, using $\lambda=10^{k}$. What are the closest values to the in-sample and out-of-sample classification errors, respectively, for k=-3? Recall that the solution for Linear Regression with Weight Decay was derived in class.

See above

Problem 4

Now, use k = 3. What are the closest values to the new in-sample and out-of-sample classification errors, respectively?

See above

Problem 5

What value of k, among the following choices, achieves the smallest out-of-sample classification error?

See above

Problem 6

What value is closest to the minimum out-of-sample classification error achieved by varying k (limiting k to integer values)?

See above

Regularization for Polynomials

Polynomial models can be viewed as linear models in a space \mathcal{Z} , under a nonlinear transform $\Phi: \mathcal{X} \to \mathcal{Z}$. Here, Φ transforms the scalar x into a vector \mathbf{z} of Legendre polynomials, $\mathbf{z} = (1, L_1(x), L_2(x), \dots, L_Q(x))$. Our hypothesis set will be expressed as a linear combination of these polynomials,

$$\mathcal{H}_Q = \left\{ h \mid h(x) = \mathbf{w}^T \mathbf{z} = \sum_{q=0}^Q w_q L_q(x) \right\},\,$$

where $L_0(x) = 1$.

Problem 7

Consider the following hypothesis set defined by the constraint:

$$\mathcal{H}(Q, C, Q_0) = \{ h \mid h(x) = \mathbf{w}^T \mathbf{z} \in \mathcal{H}_Q; w_q = C \text{ for } q \ge Q_0 \},$$

which of the following statements is correct:

- (a) $\mathcal{H}(10,0,3) \cup \mathcal{H}(10,0,4) = \mathcal{H}_4$
- (b) $\mathcal{H}(10,1,3) \cup \mathcal{H}(10,1,4) = \mathcal{H}_3$
- (c) $\mathcal{H}(10,0,3) \cap \mathcal{H}(10,0,4) = \mathcal{H}_2$
- (d) $\mathcal{H}(10,1,3) \cap \mathcal{H}(10,1,4) = \mathcal{H}_1$
- (e) None of the above

 $\mathcal{H}(10,0,3)$ is the set of all polynomials up to degree 2 (\mathcal{H}_2) , and similarly $\mathcal{H}(10,0,4)$ is the set of all polynomials up to degree 3 (\mathcal{H}_3) . Because $\mathcal{H}_2 \subset \mathcal{H}_3$, $\mathcal{H}_2 \cap \mathcal{H}_3 = \mathcal{H}_2$. Therefore the answer is (c).

Neural Networks

Problem 8

A fully connected Neural Network has $L=2; d^{(0)}=5, d^{(1)}=3, d^{(2)}=1$. If only products of the form $w_{ij}^{(l)}x_i^{(l-1)}, w_{ij}^{(l)}\delta_j^{(l)}$, and $x_i^{(l-1)}\delta_j^{(l)}$ count as operations (even for $x_0^{(l-1)}=1$), without counting anything else, which of the following is the closest to the total number of operations in a single iteration of backpropagation (using SGD on one data point)?

Let us call every 'node' in a Neural Network a unit, whether that unit is an input variable or a neuron in one of the layers. Consider a Neural Network that has 10 input units (the constant $x_0^{(0)}$ is counted here as a unit), one output unit, and 36 hidden units (each $x_0^{(l)}$ is also counted as a unit). The hidden units can be arranged in any number of layers $l = 1, \ldots, L-1$, and each layer is fully connected to the layer above it.

Problem 9

What is the minimum possible number of weights that such a network can have?

Problem 10

What is the maximum possible number of weights that such a network can have?