Comp 6321 - Machine Learning - Assignment 3

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Question 1: Midterm preparation question

Propose an adequate learning algorithm for each instance.

1.a 1000 samples, 6-dimensional continuous space, classify ∼100 examples.

1.b Clasifier for children in special-ed, justified to the board before it's implemented.

One of the easiest classification algorithms to explain in layman's terms is decision trees; since the method should be justified to the board, this would probably be an adequate choice.

1.c Binary classification of 1 million bits (empirical preference rate for others), very large data-set. Frequent updates.

1.d 40 attributes, discrete and continuous, some have noise; only about 50 labeled observations.

Question 2: Properties of entropy

2.a Compute the following for (X, Y): $p(0,0) = 1/3, p(0,1) = 1/3, p(1,0) = 0, p(1,1) = 1/3$.

i $H[x] = -\frac{1}{3}log_2\left(\frac{1}{3}\right) - \frac{2}{3}log_2\left(\frac{2}{3}\right) = .9182$

ii $H[y] = -\frac{1}{3}log_2\left(\frac{1}{3}\right) - \frac{2}{3}log_2\left(\frac{2}{3}\right) = .9182$

iii $H[y|x] = \sum_x p(x)H[Y|X=x] = \frac{2}{3}\left(-\frac{1}{2}log_2\left(\frac{1}{2}\right) - \frac{1}{2}log_2\left(\frac{1}{2}\right)\right) = \frac{2}{3}$

iv $H[x|y] = \sum_y p(x)H[X|Y=y] = \frac{2}{3}\left(-\frac{1}{2}log_2\left(\frac{1}{2}\right) - \frac{1}{2}log_2\left(\frac{1}{2}\right)\right) = \frac{2}{3}$

v $H[x,y] = 3\left(-\frac{1}{3}log_2\left(\frac{1}{3}\right)\right) = -log_2\left(\frac{1}{3}\right) = 1.5849$

vi $I[x,y] = \sum_x \sum_y p(x,y) log_2 \left(\frac{p(x,y)}{p(x)p(y)} \right) = H[x] - H[x|y] = 0.2516$

2.b Prove maximum entropy in a discrete distribution happens in U

We wish to find:

$$\arg\max_{p_n} \sum_{n=1}^{N} p_n log(p_n)$$

With constraints:

$$1 - \sum_{n=1}^{N} p_n = 0$$

We use a Lagrangian multiplier such that:

$$\nabla_{p_1,p_2,\ldots p_N} \sum_{n=1}^{N} p_n log(p_n) = \nabla_{p_1,p_2\ldots p_N} \lambda(1 - \sum_{n=1}^{N} p_n)$$

We are thus left with a system:

$$\begin{aligned}
\frac{\partial}{\partial_{p_1}} \sum_{n=1}^{N} p_n log(p_n) =& \frac{\partial}{\partial_{p_1}} \lambda(1 - \sum_{n=1}^{N} p_n) \\
\frac{\partial}{\partial_{p_2}} \sum_{n=1}^{N} p_n log(p_n) =& \frac{\partial}{\partial_{p_2}} \lambda(1 - \sum_{n=1}^{N} p_n) \\
&\vdots \\
\frac{\partial}{\partial_{p_N}} \sum_{n=1}^{N} p_n log(p_n) =& \frac{\partial}{\partial_{p_N}} \lambda(1 - \sum_{n=1}^{N} p_n) \\
1 - \sum_{n=1}^{N} p_n =& 0
\end{aligned}$$

Which in turn yields:

$$\begin{aligned}
log(p_1) + 1 =& \lambda p_1 \\
log(p_2) + 1 =& \lambda p_2 \\
&\vdots \\
log(p_N) + 1 =& \lambda p_N \\
1 - \sum_{n=1}^{N} p_n =& 0
\end{aligned}$$

From which it is clear that $p_1 = p_2 = \ldots p_N = \frac{1}{N}$, which is precisely a discrete uniform distribution.

2.c Show that T_1 wins

The notes show two possible tests for a decision tree. T1, where the left child has $[20+, 10-]$ posible outcomes in its sub-trees and the right node has $[10+, 0-]$. T2, on the other hand, yields: $left = [15+, 7-]; right = [15+, 3-]$.

The best choice should yield the maximum information gain $I[p, T_n]$,$n \in \{1, 2\}$. So for T_1:

$$\begin{aligned}
H[p] =& -\frac{1}{4}log_2\left(\frac{1}{4}\right) - \frac{3}{4}log_2\left(\frac{3}{4}\right) = 0.8112 \\
H[p|T_1 = t] =& -\frac{2}{3}log_2\left(\frac{2}{3}\right) - \frac{1}{3}log_2\left(\frac{1}{3}\right) = 0.9182 \\
H[p|T_1 = f] =& 0 \\
H[p|T_1] =& p(T_1 = t)H[p|T_1 = t] + p(T_1 = f)H[p|T_1 = f] \\
=& 0.6887 \\
I[p, T_1] =& H[p] - H[p|T_1] = 0.1225
\end{aligned}$$

Whereas for T_2 we have:

$$\begin{aligned}
H[p|T_2 = t] =& -\frac{15}{22}log_2\left(\frac{15}{22}\right) - \frac{7}{22}log_2\left(\frac{7}{22}\right) = 0.9024 \\
H[p|T_2 = f] =& -\frac{15}{18}log_2\left(\frac{15}{18}\right) - \frac{3}{18}log_2\left(\frac{3}{18}\right) = 0.65002 \\
H[p|T_2] =& p(T_2 = t)H[p|T_2 = t] + p(T_2 = f)H[p|T_2 = f] \\
=& \frac{22}{40}0.9024 + \frac{18}{40}0.65002 = 0.7888 \\
I[p, T_2] =& H[p] - H[p|T_2] = 0.02245
\end{aligned}$$

From which we can see that we gain much more information from knowing the result of T_1 than by knowing the result of T_2.

Question 3: Kernels

Suppose $k_1(\boldsymbol{x}, \boldsymbol{z})$ and $k_2(\boldsymbol{x}, \boldsymbol{z})$ are valid kernels over $\mathbb{R}^n x \mathbb{R}^n$. Prove or disprove that the following are valid kernels.

Use Mercer's theorem regarding the kernel or Gram matrix or the fact that a kernel can be expressed as $k(x, z) = \phi(\boldsymbol{x})^T \phi(\boldsymbol{z})$.

preliminaries

From Mercer, we know for each $k_1(\boldsymbol{x}, \boldsymbol{z})$ and $k_2(\boldsymbol{x}, \boldsymbol{z})$ we have corresponding kernel matrices $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ which are symmetric and positive semi-definite.

For both $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$:

Symmetry:

$$\boldsymbol{M}_i = \boldsymbol{M}_i^T \tag{1}$$

Positive semidefiniteness:

$$\boldsymbol{x}^T \boldsymbol{M}_i \boldsymbol{x} \geq 0 \tag{2}$$

$$|\boldsymbol{M}_i| \geq 0 \tag{3}$$

3.a $k(\boldsymbol{x}, \boldsymbol{z}) = ak_1(\boldsymbol{x}, \boldsymbol{z}) + bk_2(\boldsymbol{x}, \boldsymbol{z}), a, b > 0; a, b \in \mathbb{R}$

Firstly, we establish that for any valid kernel $k(\boldsymbol{x}, \boldsymbol{z}), ak(\boldsymbol{x}, \boldsymbol{z}) | a > 0; a \in \mathbb{R}$: We know that for a square matrix $\boldsymbol{A}$ of size nxn, $|a\boldsymbol{A}| = a^n |A|$., and since $a^n \geq 0 \forall n \in \mathbb{N}, a > 0$ Then the property from equation 3 holds for both of our summands. Additionally, since the scalar multiplication of a symmetric matrix yields another symmetric matrix, both summands are valid kernels.

Now, let us say:

$$ak_1(\boldsymbol{x}, \boldsymbol{z}) = k_1'(\boldsymbol{x}, \boldsymbol{z})$$

and

$$bk_2(\boldsymbol{x}, \boldsymbol{z}) = k_2'(\boldsymbol{x}, \boldsymbol{z})$$

are both valid kernels with kernel matrices $\boldsymbol{M}_1'$ and $\boldsymbol{M}_2'$. The addition of two symmetric matrices yields a symmetric matrix, so we need to check for positive semi-definiteness.

Since both $\boldsymbol{M}_1'$ and $\boldsymbol{M}_2'$ are symmetric we can write:

$$\boldsymbol{M}_1' = \boldsymbol{U}^T \boldsymbol{U}$$
$$\boldsymbol{M}_2' = \boldsymbol{V}^T \boldsymbol{V}$$

and using equation 2:

$$(\boldsymbol{x}^T \boldsymbol{U}^T \boldsymbol{U} \boldsymbol{x} + \boldsymbol{x}^T \boldsymbol{V}^T \boldsymbol{V} \boldsymbol{x}) \geq 0$$
$$\boldsymbol{x}^T (\boldsymbol{U}^T \boldsymbol{U} + \boldsymbol{V}^T \boldsymbol{V}) \boldsymbol{x} \geq 0$$
$$\boldsymbol{x}^T (\boldsymbol{M}_1' + \boldsymbol{M}_2') \boldsymbol{x} \geq 0$$

Which proves that $k(\boldsymbol{x}, \boldsymbol{z}) = ak_1(\boldsymbol{x}, \boldsymbol{z}) + bk_2(\boldsymbol{x}, \boldsymbol{z}), a, b > 0; a, b \in \mathbb{R}$ is a valid kernel.

3.b $k(\boldsymbol{x}, \boldsymbol{z}) = ak_1(\boldsymbol{x}, \boldsymbol{z}) - bk_2(\boldsymbol{x}, \boldsymbol{z}), a, b > 0; a, b \in \mathbb{R}$

Suppose:

$$a = 1, b = 1, M_1 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, M_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

Both$\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ symetric, positive semi-definite matrices. Yet $\boldsymbol{M}' = a\boldsymbol{M}_1 - b\boldsymbol{M}_2$ would yield:

$$M_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

The eigenvalues of which are $\lambda_1 = -1, \lambda_2 = 1$, making $\boldsymbol{M}'$ a non positive semi-definite matrix and thus $k(\boldsymbol{x}, \boldsymbol{z})$ is not a valid kernel.

3.c $k(\boldsymbol{x}, \boldsymbol{z}) = k_1(\boldsymbol{x}, \boldsymbol{z})k_2(\boldsymbol{x}, \boldsymbol{z})$

The kernel matrix $\boldsymbol{M'}$ of the product of two matrices $k_1(\boldsymbol{x}, \boldsymbol{z}), k_2(\boldsymbol{x}, \boldsymbol{z})$ is equivalent to the element-wise multiplication of the respective two kernel matrices $\boldsymbol{M}_1, \boldsymbol{M}_2$. This is also known as the Hadamard product or the Schur product. The Schur product theorem states that the Schur product of two positive semi-definite matrices is also positive semi-definite. It is trivial to show that symmetry is preserved under such conditions.

3.d $k(\boldsymbol{x}, \boldsymbol{z}) = f(\boldsymbol{x})f(\boldsymbol{z}), where\ f : \mathbb{R}^n \to \mathbb{R}$

Here we rely on the fact that a kernel can be expressed as $k(x, z) = \phi(\boldsymbol{x})^T\phi(\boldsymbol{z})$ where $\phi(\boldsymbol{x})$ maps $\boldsymbol{x}$ onto an n-dimensional space.

It is trivial to see that if $n = 1$ and $\phi = f$, $f(\boldsymbol{x})f(\boldsymbol{z})$ constitutes a valid kernel.

3.e $k(\boldsymbol{x}, \boldsymbol{z}) = f(\boldsymbol{x})f(\boldsymbol{z}), where\ p\ pdf.$

The same rationale as question 3.d applies here.

Question 4: Nearest neighbour vs decision trees, do boundaries coincide?

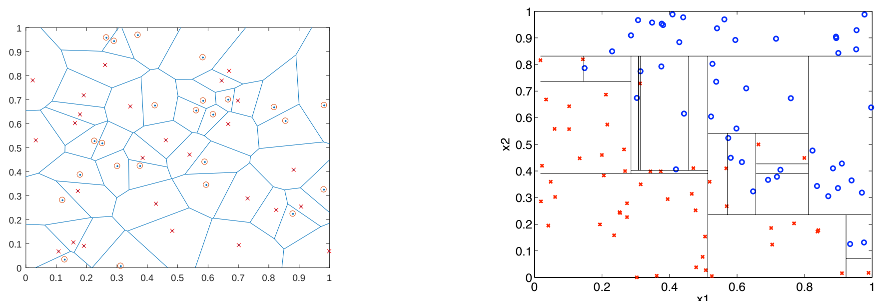
Boundaries do not necessarily coincide for these two classification strategies. In the case of trees, boundaries are composed of hyper-planes that are orthogonal to the features chosen for the separation and pass through the midpoint between neighboring points along the axis of the chosen features[1]. Thus each segment of a decision-tree boundary can have one out of d directions for a d-dimensional space[2].

Conversely, boundaries for nearest-neibours correspond to a Voronoi tessellation, where the each boundary segment corresponds to a hyper-plane running orthogonal to the line between the boundary's nearest neighbors and passing through the midpoint of such a line (thus said hyperplanes can have an any direction in the space).

For an example, see figures 1a and 1b.

[1] A combination of features can also be used, but as a crude example, if both features are chosen in a 2-d space, boundaries would yield diagonal lines.

[2] Again, a combination of features may be used but the amount of directions to choose from is still rather limited.



(a) Nearest-neighbour (b) decision tree

Figure 1: A Voronoi tessellation has boundary segments in many different directions, perpendicular to the lines between any two nearest-neighbors whereas decision-tree boundary segments are perpendicular to any one of a given set of features or feature combinations

Question 5: Bayes rate

For the following univariate case where $P(\omega_i) = \frac{1}{c}$ and

$$P(x|\omega_i) = \begin{cases} 1 & 0 \leq x \leq \frac{cr}{c-1} \\ 1 & i \leq x \leq i + 1 - \frac{cr}{c-1} \\ 0 & otherwise \end{cases}$$

5.a Show that $P^* = r$

The minimal multi-class classification error rate P^* is given by:

$$P^* = 1 - \int \arg\max_i P(\omega_i)P(x|\omega_i)dx$$

And given the class density and probability, we can see that for any region with overlapping densities, the choice of any i will maximize. Additionally, we see that the constraints imposed by existing densities demand that $0 \leq r \leq \frac{c-1}{c}$.

This in turn implies that densities overlap only in $[0, \frac{cr}{c-1}]$ Thus:

$$
\begin{aligned}
P^* =& 1 - \int P(\omega_1)P(x|\omega_1)dx \\
=& 1 - \frac{1}{c}\int_0^{\frac{cr}{c-1}} dx - \sum_{i=1}^{c}\frac{1}{c}\int_i^{i+1-\frac{cr}{c-1}} dx \\
=& 1 - \frac{1}{c}\frac{cr}{c-1} - 1 - \frac{cr}{c-1} \\
=& \frac{cr-r}{c-1} \\
=& r
\end{aligned}
$$

5.b Show the nearest-neighbor rate $P = P^*$

$$
\begin{aligned}
LNN =& \int \left[1 - \sum_{i=1}^{c} P^2(\omega_i|x)\right] p(x)dx \\
=& \int \left[1 - \sum_{i=1}^{c}\left(\frac{P(x|\omega_i)P(\omega_i)}{p(x)}\right)^2\right] p(x)dx \\
=& \int p(x) - \sum_{i=1}^{c}\frac{P(x|\omega_i)^2 P(\omega_i)^2}{p(x)} dx \\
=& \int p(x) - \sum_{i=1}^{c}\frac{P(x|\omega_i)P(\omega_i)(P(x|\omega_i)P(\omega_i))}{p(x)} dx \\
=& \int p(x) - \sum_{i=1}^{c}\frac{P(x|\omega_i)P(\omega_i)p(x)}{p(x)} dx \\
=& \int p(x)dx - \frac{1}{c}\int_0^{\frac{cr}{c-1}} dx - \sum_{i=1}^{c}\frac{1}{c}\int_i^{i+1-\frac{cr}{c-1}} dx \\
=& 1 - \frac{1}{c}\frac{cr}{c-1} - 1 - \frac{cr}{c-1} \\
=& \frac{cr-r}{c-1} \\
=& r
\end{aligned}
$$

Question 6: Implementation