Area Under the ROC Curve

1. Let $\boldsymbol{X} \in \mathbb{R}^d$ be a random vector and let $Y \in \{0, 1\}$ be a random variable.

2. Let $p(\boldsymbol{x}, y)$ denote the joint distribution of $\boldsymbol{X}$ and Y, let $p(y \mid \boldsymbol{x})$ denote the conditional distribution of Y given $\boldsymbol{X}$, and let $p(\boldsymbol{x} \mid y)$ denote the conditional distribution of $\boldsymbol{X}$ given Y.

3. Let $q(y \mid \boldsymbol{x})$ be a model of $p(y \mid \boldsymbol{x})$.

4. Let $f(q \mid y)$ and $F(q \mid y)$ denote the probability density function and cumulative distribution function, respectively, of the random variable $q(0 \mid \boldsymbol{X})$ with respect to $p(\boldsymbol{x} \mid y)$.

5. The ROC curve is the curve that results from plotting the 2-dimensional points

$$(F(q \mid 0), F(q \mid 1)), \quad q \in [0, 1]$$

6. Consider the following process:

   1. Draw independent samples $\boldsymbol{x}_0 \sim p(\boldsymbol{x} \mid 0)$ and $\boldsymbol{x}_1 \sim p(\boldsymbol{x} \mid 1)$.
   2. Compute $q_0 = q(0 \mid \boldsymbol{x}_0)$ and $q_1 = q(0 \mid \boldsymbol{x}_1)$.

   In other words, draw independent samples $q_0 \sim f(q \mid 0)$ and $q_1 \sim f(q \mid 1)$. We are interested in the probability that $q_1 < q_0$ which is equivalent to the joint probability that $q_1 < q$ and $q_0 = q$ for some $q \in [0, 1]$ — that is,

$$\int_0^1 F(q \mid 1) f(q \mid 0) dq = \int_0^1 F(q \mid 1) dF(q \mid 0)$$

   which is the area under the ROC curve (i.e., AUC).

7. Let $\left(\boldsymbol{x}_1^{(0)}, 0\right), \ldots, \left(\boldsymbol{x}_{n_0}^{(0)}, 0\right), \left(\boldsymbol{x}_1^{(1)}, 1\right), \ldots, \left(\boldsymbol{x}_{n_1}^{(1)}, 1\right)$ be an i.i.d. sample drawn from $p(\boldsymbol{x}, y)$.

8. For each $\left(\boldsymbol{x}_{i_j}^{(j)}, j\right)$, compute $q_{i_j}^{(j)} = q\left(0 \mid \boldsymbol{x}_{i_j}^{(j)}\right)$.

9. For each $q_{i_0}^{(0)}$, compute the number of $q_{i_1}^{(1)}$ such that $q_{i_1}^{(1)} < q_{i_0}^{(0)}$ and let c_{i_0} denote the count.

10. It follows that AUC with respect to the empirical distributions of our sample is given by

$$\widehat{\text{AUC}} = \sum_{k=1}^{n_0} \left(\frac{c_k}{n_1}\right) \left(\frac{1}{n_0}\right)$$

11. If we sort the $q_{i_j}^{(j)}$ in ascending order and let r_k denote the rank of the k^{th} $q_{i_0}^{(0)}$, then $c_k = r_k - k$ and, hence,

$$\widehat{\text{AUC}} = \frac{1}{n_0 n_1} \sum_{k=1}^{n_0} (r_k - k) = \frac{1}{n_0 n_1} \left(R - \frac{n_0(n_0 + 1)}{2}\right)$$

   where R denotes the sum of the ranks of the $q_{i_0}^{(0)}$.

References

1. Hand, D. J., & Till, R. J. (2001). A Simple Generalisation of the Area Under the ROC Curve for Multiple Class Classification Problems. Machine learning, 45(2), 171-186.