Machine Learning — Statistical Methods for Machine Learning Risk Analysis for Nearest-Neighbor

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version of May 31, 2023

We investigate the problem of bounding the zero-one loss risk of the 1-NN binary classifier averaged with respect to the random draw of the training set. Under some assumptions on the data distribution \mathcal{D} , we prove a bound of the form

$$\mathbb{E}\left[\ell_{\mathcal{D}}(A(S_m))\right] \le 2\,\ell_{\mathcal{D}}(f^*) + \varepsilon_m \tag{1}$$

where A denotes the 1-NN algorithm, S_m the training set of size m, $\ell_{\mathcal{D}}(f^*)$ is the Bayes risk, and ε_m is a quantity that vanishes for $m \to \infty$. Note that we are able to compare $\mathbb{E}[\ell_{\mathcal{D}}(A(S_m))]$ directly to the Bayes risk, showing that 1-NN is—in some sense—a powerful learning algorithm.

Recall that in binary classification we denote the joint distribution of (\boldsymbol{X}, Y) with the pair (\mathcal{D}_X, η) , where \mathcal{D}_X is the marginal of \mathcal{D} on \boldsymbol{X} and $\eta(\boldsymbol{x}) = \mathbb{P}(Y = 1 | \boldsymbol{X} = \boldsymbol{x})$. Fix m and let $S = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$ be a training set of size m. we define the map $\pi(S, \cdot) : \mathbb{R}^d \to \{1, \ldots, m\}$ by

$$\pi(S, \boldsymbol{x}) = \operatorname*{argmin}_{t=1, \dots, m} \|\boldsymbol{x} - \boldsymbol{x}_t\| .$$

If there is more than one point \boldsymbol{x}_t achieving the minimum in the above expression, then $\pi(S, \boldsymbol{x})$ selects one of them using any deterministic tie-breaking rule; our analysis does not depend on the specific rule being used. The 1-NN classifier $h_S = A(S)$ is defined by $h_S(\boldsymbol{x}) = y_{\pi(S,\boldsymbol{x})}$.

From now on, the training set S is a sample $\{(X_1, Y_1), \ldots, (X_m, Y_m)\}$ drawn i.i.d. from \mathcal{D} . The expected risk is defined by

$$\mathbb{E}\big[\ell_{\mathcal{D}}\big(A(S)\big)\big] = \mathbb{P}\Big(Y_{\pi(S,\boldsymbol{X})} \neq Y\Big)$$

Where probabilities and expectations are understood with respect to the random draw of training set S and of the example (\mathbf{X}, Y) with respect to which the risk of A(S) is computed.

We now state a crucial lemma.

Lemma 1. The expected risk of the 1-NN classifier can be written as follows

$$\mathbb{E}\left[\ell_{\mathcal{D}}(h_{S})\right] = \mathbb{E}\left[\eta\left(\boldsymbol{X}_{\pi(S,\boldsymbol{X})}\right)\left(1-\eta(\boldsymbol{X})\right)\right] + \mathbb{E}\left[\left(1-\eta\left(\boldsymbol{X}_{\pi(S,\boldsymbol{X})}\right)\right)\eta(\boldsymbol{X})\right]$$

To proceed with the analysis, we now need some assumptions on D_X and η . First, all data points X drawn from D_X satisfy $\max_i |X_i| \leq 1$ with probability one. In other words, $X \in [-1, 1]^d$ with probability 1. Let $\mathcal{X} \equiv [-1, 1]^d$ the subsets of data points with this property. Second we assume that η is Lipschitz on \mathcal{X} with constant c > 0. We can thus write

$$\eta(\boldsymbol{x}') \le \eta(\boldsymbol{x}) + c \left\| \boldsymbol{x} - \boldsymbol{x}' \right\|$$
(2)

$$1 - \eta(\boldsymbol{x}') \le 1 - \eta(\boldsymbol{x}) + c \left\| \boldsymbol{x} - \boldsymbol{x}' \right\|$$
(3)

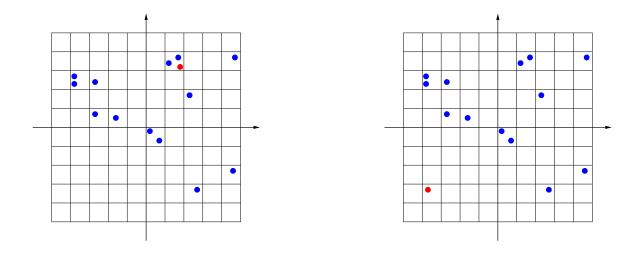


Figure 1: Bidimensional example of the construction used in the analysis of 1-NN. Left pane: X (the red point) is in the same square C_i as its closest training point $X_{\pi(S,X)}$. Hence, $||X - X_{\pi(S,X)}||$ is bounded by the length of the diagonal of this square. Right pane: here there are no training points in the square where X lies. Hence, $||X - X_{\pi(S,X)}||$ can only be bounded by the length of the entire data space (the large square).

Using (2) and (3), for all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{X}$ we have

$$\begin{split} \eta(\boldsymbol{x}) \big(1 - \eta(\boldsymbol{x}') \big) &+ \big(1 - \eta(\boldsymbol{x}) \big) \eta(\boldsymbol{x}') \\ &\leq \eta(\boldsymbol{x}) \big(1 - \eta(\boldsymbol{x}) \big) + \eta(\boldsymbol{x}) c \, \big\| \boldsymbol{x} - \boldsymbol{x}' \big\| + \big(1 - \eta(\boldsymbol{x}) \big) \eta(\boldsymbol{x}) + \big(1 - \eta(\boldsymbol{x}) \big) c \, \big\| \boldsymbol{x} - \boldsymbol{x}' \big\| \\ &= 2\eta(\boldsymbol{x}) \big(1 - \eta(\boldsymbol{x}) \big) + c \, \big\| \boldsymbol{x} - \boldsymbol{x}' \big\| \\ &\leq 2 \min \big\{ \eta(\boldsymbol{x}), 1 - \eta(\boldsymbol{x}) \big\} + c \, \big\| \boldsymbol{x} - \boldsymbol{x}' \big\| \end{split}$$

where the last inequality holds because $z(1-z) \leq \min\{z, 1-z\}$ for all $z \in [0,1]$. Therefore

$$\mathbb{E}\big[\ell_{\mathcal{D}}(h_S)\big] \leq 2 \mathbb{E}\Big[\min\big\{\eta(\boldsymbol{X}), 1 - \eta(\boldsymbol{X})\big\}\Big] + c \mathbb{E}\big[\left\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\right\|\big] \ .$$

Recalling that the Bayes risk for the zero-one loss is $\ell_{\mathcal{D}}(f^*) = \mathbb{E}\left[\min\{\eta(\boldsymbol{X}), 1 - \eta(\boldsymbol{X})\}\right]$ we have

$$\mathbb{E}\left[\ell_{\mathcal{D}}(h_S)\right] \leq 2\,\ell_{\mathcal{D}}(f^*) + c\,\mathbb{E}\left[\left\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\right\|\right]\,.$$

In order to bound the term containing the expected value of $\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\|$ we partition the data space \mathcal{X} in *d*-dimensional hypercubes with side $\varepsilon > 0$, see Figure 1 for a bidimensional example. Let C_1, \ldots, C_r the resulting hypercubes. We can now bound $\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\|$ using a case analysis. Assume first that \boldsymbol{X} belongs to a C_i in which there is at least a training point \boldsymbol{X}_t . Then $\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\|$ is at most the length of the diagonal of the hypercube, which is $\varepsilon\sqrt{d}$, see the left pane in Figure 1. Now assume that \boldsymbol{X} belongs to a C_i in which there are no training points. Then $\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\|$ is only bounded by the length of the diagonal of \mathcal{X} , which is $2\sqrt{d}$, see the

right pane in Figure 1. Hence, we may write

$$\mathbb{E}\Big[\left\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\right\|\Big] \leq \mathbb{E}\left[\varepsilon\sqrt{d}\sum_{i=1}^{r}\mathbb{I}\{C_{i}\cap S\neq\emptyset\}\mathbb{I}\{\boldsymbol{X}\in C_{i}\} + 2\sqrt{d}\sum_{i=1}^{r}\mathbb{I}\{C_{i}\cap S=\emptyset\}\mathbb{I}\{\boldsymbol{X}\in C_{i}\}\right]$$
$$= \varepsilon\sqrt{d}\,\mathbb{E}\left[\sum_{i=1}^{r}\mathbb{I}\{C_{i}\cap S\neq\emptyset\}\mathbb{I}\{\boldsymbol{X}\in C_{i}\}\right] + 2\sqrt{d}\sum_{i=1}^{r}\mathbb{E}\left[\mathbb{I}\{C_{i}\cap S=\emptyset\}\mathbb{I}\{\boldsymbol{X}\in C_{i}\}\right]$$

where in the last step we used linearity of the expected value. Now observe that, for all S and X,

$$\sum_{i=1}^{r} \mathbb{I}\{C_i \cap S \neq \emptyset\} \mathbb{I}\{\mathbf{X} \in C_i\} \in \{0, 1\}$$

because $X \in C_i$ for only one $i = 1, \ldots, d$. Therefore,

$$\mathbb{E}\left[\sum_{i=1}^{r} \mathbb{I}\{C_i \cap S \neq \emptyset\} \mathbb{I}\{\boldsymbol{X} \in C_i\}\right] \leq 1 \; .$$

To bound the remaining term, we use the independence between \boldsymbol{X} and the training set S,

$$\mathbb{E}\left[\mathbb{I}\{C_i \cap S = \emptyset\}\mathbb{I}\{\mathbf{X} \in C_i\}\right] = \mathbb{E}\left[\mathbb{I}\{C_i \cap S = \emptyset\}\right]\mathbb{E}\left[\mathbb{I}\{\mathbf{X} \in C_i\}\right] = \mathbb{P}\left(C_i \cap S = \emptyset\right)\mathbb{P}\left(\mathbf{X} \in C_i\right) \ .$$

Since S contains m data points independently drawn, for a generic data point X' we have that

$$\mathbb{P}(C_i \cap S = \emptyset) = (1 - \mathbb{P}(\mathbf{X}' \in C_i))^m \le \exp(-m\mathbb{P}(\mathbf{X}' \in C_i))$$

where in the last step we used the inequality $(1-p)^m \leq e^{-pm}$. Setting $p_i = \mathbb{P}(\mathbf{X}' \in C_i)$ we have

$$\mathbb{E}\Big[\| \mathbf{X} - \mathbf{X}_{\pi(S,\mathbf{X})} \| \Big] \le \varepsilon \sqrt{d} + \left(2\sqrt{d} \right) \sum_{i=1}^{r} e^{-p_i m} p_i$$
$$\le \varepsilon \sqrt{d} + \left(2\sqrt{d} \right) \sum_{i=1}^{r} \max_{0 \le p \le 1} e^{-pm} p$$
$$= \varepsilon \sqrt{d} + \left(2\sqrt{d} \right) r \max_{0 \le p \le 1} e^{-pm} p .$$

The concave function $g(p) = e^{-pm}p$ is maximized for $p = \frac{1}{m}$. Therefore,

$$\mathbb{E}\Big[\left\|\boldsymbol{X} - \boldsymbol{X}_{\pi(S,\boldsymbol{X})}\right\|\Big] \le \varepsilon\sqrt{d} + \left(2\sqrt{d}\right)\frac{r}{em} = \sqrt{d}\left(\varepsilon + \frac{2}{em}\left(\frac{2}{\varepsilon}\right)^{d}\right)$$

where we used the fact that the number r of hypercubes is equal to $\left(\frac{2}{\varepsilon}\right)^d$. Putting evertything together we find that

$$\mathbb{E}\left[\ell_{\mathcal{D}}(h_S)\right] \le 2\,\ell_{\mathcal{D}}(f^*) + c\,\sqrt{d}\left(\varepsilon + \frac{2}{em}\left(\frac{2}{\varepsilon}\right)^d\right)$$

Since this holds for all $0 < \varepsilon < 1$, we can set $\varepsilon = 2 m^{-1/(d+1)}$. This gives

$$\varepsilon + \frac{2}{em} \left(\frac{2}{\varepsilon}\right)^d = 2m^{-1/(d+1)} + \frac{2^{d+1}2^{-d}m^{d/(d+1)}}{em} = 2m^{-1/(d+1)} \left(1 + \frac{1}{e}\right) \le 4m^{-1/(d+1)} .$$
(4)

Substituting this bound in (4), we finally obtain

$$\mathbb{E}\big[\ell_{\mathcal{D}}(h_S)\big] \le 2\,\ell_{\mathcal{D}}(f^*) + c\,4m^{-1/(d+1)}\sqrt{d}\;.$$

Note that for $m \to \infty$, $\ell_{\mathcal{D}}(f^*) \leq \mathbb{E}[\ell_{\mathcal{D}}(h_S)] \leq 2 \ell_{\mathcal{D}}(f^*)$. Namely, the asymptotic risk of 1-NN lies between the Bayes risk and twice the Bayes risk.