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

Instructor: Nicolò Cesa-Bianchi
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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

$$
\begin{equation*}
\mathbb{E}\left[\ell_{\mathcal{D}}\left(A\left(S_{m}\right)\right)\right] \leq 2 \ell_{\mathcal{D}}\left(f^{*}\right)+\varepsilon_{m} \tag{1}
\end{equation*}
$$

where $A$ denotes the 1-NN algorithm, $S_{m}$ the training set of size $m, \ell_{\mathcal{D}}\left(f^{*}\right)$ is the Bayes risk, and $\varepsilon_{m}$ is a quantity that vanishes for $m \rightarrow \infty$. Note that we are able to compare $\mathbb{E}\left[\ell_{\mathcal{D}}\left(A\left(S_{m}\right)\right)\right]$ 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 $\left(\mathcal{D}_{X}, \eta\right)$, where $\mathcal{D}_{X}$ is the marginal of $\mathcal{D}$ on $\boldsymbol{X}$ and $\eta(\boldsymbol{x})=\mathbb{P}(Y=1 \mid \boldsymbol{X}=\boldsymbol{x})$. Fix $m$ and let $S=$ $\left\{\left(\boldsymbol{x}_{1}, y_{1}\right), \ldots,\left(\boldsymbol{x}_{m}, y_{m}\right)\right\}$ be a training set of size $m$. we define the map $\pi(S, \cdot): \mathbb{R}^{d} \rightarrow\{1, \ldots, m\}$ by

$$
\pi(S, \boldsymbol{x})=\underset{t=1, \ldots, m}{\operatorname{argmin}}\left\|\boldsymbol{x}-\boldsymbol{x}_{t}\right\| .
$$

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 $\left\{\left(\boldsymbol{X}_{1}, Y_{1}\right), \ldots,\left(\boldsymbol{X}_{m}, Y_{m}\right)\right\}$ drawn i.i.d. from $\mathcal{D}$. The expected risk is defined by

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

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

We now state a crucial lemma.
Lemma 1. The expected risk of the $1-N N$ classifier can be written as follows

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

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

$$
\begin{align*}
\eta\left(\boldsymbol{x}^{\prime}\right) & \leq \eta(\boldsymbol{x})+c\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\|  \tag{2}\\
1-\eta\left(\boldsymbol{x}^{\prime}\right) & \leq 1-\eta(\boldsymbol{x})+c\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\| \tag{3}
\end{align*}
$$



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

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

$$
\begin{aligned}
& \eta(\boldsymbol{x})\left(1-\eta\left(\boldsymbol{x}^{\prime}\right)\right)+(1-\eta(\boldsymbol{x})) \eta\left(\boldsymbol{x}^{\prime}\right) \\
& \quad \leq \eta(\boldsymbol{x})(1-\eta(\boldsymbol{x}))+\eta(\boldsymbol{x}) c\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\|+(1-\eta(\boldsymbol{x})) \eta(\boldsymbol{x})+(1-\eta(\boldsymbol{x})) c\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\| \\
& \quad=2 \eta(\boldsymbol{x})(1-\eta(\boldsymbol{x}))+c\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\| \\
& \quad \leq 2 \min \{\eta(\boldsymbol{x}), 1-\eta(\boldsymbol{x})\}+c\left\|\boldsymbol{x}-\boldsymbol{x}^{\prime}\right\|
\end{aligned}
$$

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

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

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

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

In order to bound the term containing the expected value of $\left\|\boldsymbol{X}-\boldsymbol{X}_{\pi(S, \boldsymbol{X})}\right\|$ 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 $\left\|\boldsymbol{X}-\boldsymbol{X}_{\pi(S, \boldsymbol{X})}\right\|$ 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 $\left\|\boldsymbol{X}-\boldsymbol{X}_{\pi(S, \boldsymbol{X})}\right\|$ 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 $\left\|\boldsymbol{X}-\boldsymbol{X}_{\pi(S, \boldsymbol{X})}\right\|$ 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

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

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

$$
\sum_{i=1}^{r} \mathbb{I}\left\{C_{i} \cap S \neq \emptyset\right\} \mathbb{I}\left\{\boldsymbol{X} \in C_{i}\right\} \in\{0,1\}
$$

because $\boldsymbol{X} \in C_{i}$ for only one $i=1, \ldots, d$. Therefore,

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

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

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

Since $S$ contains $m$ data points independently drawn, for a generic data point $\boldsymbol{X}^{\prime}$ we have that

$$
\mathbb{P}\left(C_{i} \cap S=\emptyset\right)=\left(1-\mathbb{P}\left(\boldsymbol{X}^{\prime} \in C_{i}\right)\right)^{m} \leq \exp \left(-m \mathbb{P}\left(\boldsymbol{X}^{\prime} \in C_{i}\right)\right)
$$

where in the last step we used the inequality $(1-p)^{m} \leq e^{-p m}$. Setting $p_{i}=\mathbb{P}\left(\boldsymbol{X}^{\prime} \in C_{i}\right)$ we have

$$
\begin{aligned}
\mathbb{E}\left[\left\|\boldsymbol{X}-\boldsymbol{X}_{\pi(S, \boldsymbol{X})}\right\|\right] & \leq \varepsilon \sqrt{d}+(2 \sqrt{d}) \sum_{i=1}^{r} e^{-p_{i} m} p_{i} \\
& \leq \varepsilon \sqrt{d}+(2 \sqrt{d}) \sum_{i=1}^{r} \max _{0 \leq p \leq 1} e^{-p m} p \\
& =\varepsilon \sqrt{d}+(2 \sqrt{d}) r \max _{0 \leq p \leq 1} e^{-p m} p
\end{aligned}
$$

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

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

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

$$
\mathbb{E}\left[\ell_{\mathcal{D}}\left(h_{S}\right)\right] \leq 2 \ell_{\mathcal{D}}\left(f^{*}\right)+c \sqrt{d}\left(\varepsilon+\frac{2}{e m}\left(\frac{2}{\varepsilon}\right)^{d}\right)
$$

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

$$
\begin{equation*}
\varepsilon+\frac{2}{e m}\left(\frac{2}{\varepsilon}\right)^{d}=2 m^{-1 /(d+1)}+\frac{2^{d+1} 2^{-d} m^{d /(d+1)}}{e m}=2 m^{-1 /(d+1)}\left(1+\frac{1}{e}\right) \leq 4 m^{-1 /(d+1)} . \tag{4}
\end{equation*}
$$

Substituting this bound in (4), we finally obtain

$$
\mathbb{E}\left[\ell_{\mathcal{D}}\left(h_{S}\right)\right] \leq 2 \ell_{\mathcal{D}}\left(f^{*}\right)+c 4 m^{-1 /(d+1)} \sqrt{d} .
$$

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

