OPTIMAL CHOICE OF $k$ FOR $k$-NEAREST NEIGHBOR REGRESSION

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ABSTRACT. The $k$-nearest neighbor algorithm ($k$-NN) is a widely used non-parametric method for classification and regression. Finding the optimal $k$ in $k$-NN regression on a given dataset is a problem that has received considerable attention in the literature. A number of practical algorithms for solving this problem have been suggested recently. The main result of this paper is that the value of $k$ obtained by the simple and quick leave-one-out cross-validation (LOOCV) procedure is optimal under fairly general conditions.

1. Introduction

Non-parametric regression is an important problem in statistics and machine learning [17, 27, 30]. The $k$-nearest neighbors algorithm ($k$-NN) is a popular non-parametric method of classification and regression. For a given sample of $n$ pairs $(x_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ and a point $x \in \mathbb{R}^d$ the $k$-NN algorithm outputs

$$\hat{y} = \hat{m}_{k,n}(x) = \frac{1}{k} \sum_{j \in N_k(x)} y_j$$

(1.1)

as an estimate of $m(x) := \mathbb{E}[y \mid x]$, where $N_k(x)$ is the set of indices of the $k$ nearest neighbors of $x$ among the $x_i$'s and $\mathbb{E}[y \mid x]$ denotes the expected value of the response given that the vector of predictors equals $x$.

The $k$-NN estimator with a fixed value of $k$ was analyzed in [5]. When $k$ is fixed, the $k$-NN estimator is not consistent. Consistency can be expected only when $k \to \infty$ as $n \to \infty$. The first results in this direction were obtained in [25], and subsequently improved in [8, 9]. Asymptotic normality was studied in [20].

The variance of the $k$-NN estimator typically decreases as $k$ grows, whereas the bias increases. This suggests that in a given problem, there is an optimal choice of $k$ which gives the minimum mean squared error. The problem of finding the best growth rate of $k$ and the convergence rate of the corresponding estimator has attracted considerable attention in the literature [1, 2, 4, 7, 10, 13, 14, 16, 20, 21, 23]. As a result of these efforts, the theoretically optimal value of $k$ is now quite well-understood in various

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circumstances. But from a practical point of view, these results are hard to implement. This is because the theoretically optimal choice of $k$ often involves knowledge that is not available to the user. For example, it usually involves the error variance, but we cannot get our hands on it before solving the regression problem.

To circumvent such issues, various interesting ways of estimating the optimal $k$ from the data have been suggested in recent years \cite{3, 12, 31, 32}. The main contribution of this paper is a non-asymptotic error bound which shows that a very old and simple method of choosing $k$ by a certain kind of cross-validation, known as leave-one-out cross-validation (LOOCV), is able to estimate the optimal $k$ quickly and efficiently. The consistency of this procedure has been known for a long time \cite{22}, but the fact that this method is actually able to produce the optimal $k$ was not known before.

2. Main result

Let $x$ be a $d$-dimensional random vector and

$$y = m(x) + \epsilon,$$

where $m : \mathbb{R}^d \to \mathbb{R}$ is a measurable function and $\epsilon$ is a mean-zero random variable that is independent of $x$. Let $\mu := m(x)$. Assume that there are finite constants $K_1$ and $K_2$ such that $\mathbb{E}(\epsilon^2/K_1)$ and $\mathbb{E}(\epsilon^2/K_2)$ are bounded by 2.

Let $(x_1, y_1), \ldots, (x_n, y_n)$ be i.i.d. copies of $(x, y)$. This is our dataset. For each $i$, let $N_k(i)$ be the indices of the $k$ nearest neighbors of $x_i$ among $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n$, where ties be broken at random. Define

$$\hat{m}_{k,n}(x_i) := 1/k \sum_{j \in N_k(i)} y_j,$$

and let

$$\text{MSE}(k) := \mathbb{E}[(m(x_i) - \hat{m}_{k,n}(x_i))^2],$$

noting that the right side does not actually depend on $i$ due to the i.i.d. nature of the data. We will say that $\text{MSE}(k)$ is the mean squared error of $k$-NN regression on this dataset. Our main object of interest is the number

$$k^* := \arg\min_{1 \leq k \leq n-1} \text{MSE}(k).$$

Of course, we cannot directly compute $k^*$ from the data since the function $m$ is unknown. Instead, we produce a surrogate. Define

$$f(k) := \frac{1}{n} \sum_{i=1}^n \left( y_i - \frac{1}{k} \sum_{j \in N_k(i)} y_j \right)^2,$$

and let

$$\tilde{k} := \arg\min_{1 \leq k \leq n-1} f(k).$$
Note that $\tilde{k}$, unlike $k^*$, is computed from the data. The intention is to use $\tilde{k}$ as the chosen value of $k$ in $k$-NN regression. This procedure for selecting $k$ is known as leave-one-out cross-validation (LOOCV). The following theorem, which is the main result of this paper, shows that

$$|\text{MSE}(k^*) - \text{MSE}(\tilde{k})| = O\left(\sqrt{\frac{\log n}{n}}\right)$$

when $C$, $K$ and $d$ are fixed and $n \to \infty$. One of the main strengths of this theorem is that no other condition is needed.

**Theorem 2.1.** Let $K_1$, $K_2$, $k^*$ and $\tilde{k}$ be as above. Then there are positive constants $A$ and $B$ depending on $d$, $K_1$ and $K_2$, such that for any $t \geq 0$,

$$P(|\text{MSE}(k^*) - \text{MSE}(\tilde{k})| \geq t) \leq 4ne^{-n \min\{At^2, Bt\}} + 4ne^{-n}.$$

A remarkable consequence of the above theorem is that the choice of $k$ by LOOCV adapts automatically to the smoothness of the regression function $m$, because the bound on the right does not depend on the smoothness of $m$.

In many situations, $\text{MSE}(k^*)$ is much greater than $n^{-1/2}(\log n)^{1/2}$. For example, by [17, Theorem 3.2], for Lipschitz functions with bounded support, the lower minimax rate of convergence (in terms of MSE) is $O(n^{-2/(2+d)})$ and for $d \geq 3$. In such cases, this result implies that $\text{MSE}(k^*)/\text{MSE}(\tilde{k}) \to 1$ as $n \to \infty$.

3. Proof

For a matrix $A$, recall that the 2-norm $\|A\|_2$ and the Frobenius norm $\|A\|_F$ are defined as

$$\|A\|_2 = \sup_{\|x\|=1} \|Ax\|, \quad \|A\|_F = \left(\sum_{i,j} a_{ij}^2\right)^{1/2}.$$

Throughout this proof, $\gamma_d$ will denote any constant that depends only on $d$. The value of $\gamma_d$ may change from line to line.

Let $\mu_i := m(x_i)$. By writing $y_i = \mu_i + \epsilon_i$, we have

$$f(k) = \frac{1}{n} \sum_{i=1}^n \left( y_i - \frac{1}{k} \sum_{j \not\in N_k(i)} y_j \right)^2$$

$$= \frac{1}{n} \sum_{i=1}^n \left( \mu_i + \epsilon_i - \frac{1}{k} \sum_{j \not\in N_k(i)} y_j \right)^2$$

$$= \frac{1}{n} \sum_{i=1}^n \left[ \left( \mu_i - \frac{1}{k} \sum_{j \not\in N_k(i)} y_j \right)^2 + \epsilon_i^2 + 2\epsilon_i \left( \mu_i - \frac{1}{k} \sum_{j \not\in N_k(i)} y_j \right) \right].$$
Since the \( \epsilon_i \)'s are independent with mean zero, taking expectation on both sides gives
\[
\mathbb{E}[f(k)] = \mathbb{E}[\epsilon^2] + \text{MSE}(k).
\] (3.1)

Define \( g(k) := \mathbb{E}[f(k)] \). By definition of \( k^* \), \( \text{MSE}(k^*) \leq \text{MSE}(k) \) for all \( k \).
In particular, \( \text{MSE}(k^*) \leq \text{MSE}(\tilde{k}) \), which implies that \( g(k^*) \leq g(\tilde{k}) \). Also
by definition of \( \tilde{k} \), we have \( f(\tilde{k}) \leq f(k^*) \). Putting these two together, we get
\[
\mathbb{P}(|\text{MSE}(k^*) - \text{MSE}(\tilde{k})| \geq t) = \mathbb{P}(g(\tilde{k}) - g(k^*) \geq t) \\
\leq \mathbb{P}(g(\tilde{k}) - g(k^*) \geq t + f(\tilde{k}) - f(k^*)) \\
\leq \mathbb{P}(|g(k^*) - f(k^*)| \geq t/2) + \mathbb{P}(|g(\tilde{k}) - f(\tilde{k})| \geq t/2) \\
\leq 2 \sum_{k=1}^{n-1} \mathbb{P}(|f(k) - g(k)| \geq t/2).
\]
Thus, the proof will be complete if we can prove the following lemma.

**Lemma 3.1.** There are positive constants \( A \) and \( B \) depending on \( d \), \( K_1 \) and \( K_2 \) such that for any \( 1 \leq k \leq n - 1 \) and any \( t > 0 \),
\[
\mathbb{P}(|f(k) - g(k)| \geq t) \leq 2e^{-n \min\{At^2, Bt\}} + 2e^{-n}.
\]

Define a nonsymmetric \( n \times n \) matrix \( B = [b_{ij}] \) as
\[
b_{ij} := \begin{cases} 
1 & i = j, \\
0 & j \not\in N_k(i), \\
-1/k & j \in N_k(i).
\end{cases}
\] (3.2)

Let \( A = [a_{ij}] = B^T B / n \). Also let \( \epsilon = (\epsilon_1, \ldots, \epsilon_n) \) and \( \mu = (\mu_1, \ldots, \mu_n) \).
Then we can rewrite \( f(k) \) in the following form:
\[
f(k) = (\epsilon + \mu)^T A (\epsilon + \mu).
\] (3.3)

Using the triangle inequality, we have
\[
|f(k) - g(k)| = |\epsilon^T A \epsilon - \mathbb{E}[\epsilon^T A \epsilon] + 2\epsilon^T A \mu| \\
\leq |\epsilon^T A \epsilon - \mathbb{E}[\epsilon^T A \epsilon]| + 2|\epsilon^T A \mu|.
\]
Therefore it’s enough to find probability tail bounds on \( |\epsilon^T A \epsilon - \mathbb{E}[\epsilon^T A \epsilon]| \) and \( |\epsilon^T A \mu| \). To find such bounds we need to have bounds on the Frobenius norm and the 2-norm of \( A \). The following lemmas give such bounds.

**Lemma 3.2.** For the matrix \( A \) defined above,
\[
\|A\|_F^2 \leq \frac{\gamma_d}{n},
\] (3.4)
where \( \gamma_d \) is a constant that only depends on \( d \).
Lemma 3.3. For the matrix \( A \) defined above,

\[ \| A \|_2 \leq \frac{\gamma_d}{n}, \tag{3.5} \]

where \( \gamma_d \) is a constant that only depends on \( d \).

We will prove these lemmas later.

**Proof of Lemma 3.1** Throughout this proof, \( P' \) and \( E' \) denotes probability and expectation conditional on \( x_1, \ldots, x_n \). As usual, \( \gamma_d \) denotes any constant that depends only on \( d \), and \( c \) will denote any universal constant. First, let us obtain a tail bound for \( |e^T A e - E[e^T A e]| \). By the Hanson–Wright inequality [24] and Lemmas 3.2 and 3.3, we have

\[
P'(|e^T A e - E[e^T A e]| \geq t) \leq 2 \exp \left( -c \min \left\{ \frac{t^2}{K_1^2 \| A \|^2_2}, \frac{t}{K_1 \| A \|_2} \right\} \right).
\]

An easy computation gives

\[
E'[e^T A e] = \frac{1}{n} \sum_{i=1}^{n} E \left( \epsilon_i - \frac{1}{k} \sum_{j \in N_k(i)} \epsilon_j \right)^2
= \left( 1 + \frac{1}{k} \right) E(\epsilon^2). \tag{3.7}
\]

The right side of (3.7) does not depend on \( x_1, \ldots, x_n \). Therefore

\[
E'[e^T A e] = E[e^T A e]. \tag{3.8}
\]

Putting (3.8) and (3.6) together gives us

\[
P'(|e^T A e - E[e^T A e]| \geq t) = P'(|e^T A e - E'[e^T A e]| \geq t)
\leq 2 \exp \left( -n \min \left\{ \frac{t^2}{K_1^2 \gamma_d}, \frac{t}{K_1 \gamma_d} \right\} \right). \tag{3.9}
\]

Since the right side of (3.9) does not depend on \( x_1, \ldots, x_n \), we get

\[
P(|e^T A e - E[e^T A e]| \geq t) \leq 2 \exp \left( -n \min \left\{ \frac{t^2}{K_1^2 \gamma_d}, \frac{t}{K_1 \gamma_d} \right\} \right) \tag{3.10}
\]

Next, we obtain a tail bound for \( |e^T A \mu| \). Remember that \( E[\epsilon_i^2/K_1] \leq 2 \) and therefore \( \epsilon_i \)'s are sub-Gaussian. Then by the equivalent properties of sub-Gaussian random variables [28], there exist a constant \( C_1 \) that only depends on \( K_1 \) such that \( E[\epsilon^2] \leq e^{\lambda^2 C_1/2} \) for all \( \lambda \). Then by using the Hoeffding
bound for sub-Gaussian variables \[29\), Proposition 2.5], we have

\[ P'(\|e^T A \mu\| \geq t) = P\left( \left| \sum_{j=1}^{n} \left( \sum_{i=1}^{n} a_{ji} \mu_i \right) \epsilon_j \right| \geq t \right) \leq 2 \exp \left( - \frac{t^2}{2C_1 \sum_{j=1}^{n} (\sum_{i=1}^{n} a_{ji} \mu_i)^2} \right). \tag{3.11} \]

Note that

\[ \sum_{j=1}^{n} \left( \sum_{i=1}^{n} a_{ji} \mu_j \right)^2 \leq \|A\|_F^2 \|\mu\|^2. \tag{3.12} \]

Inequalities (3.11) and (3.12) together give

\[ P'(\|e^T A \mu\| \geq t) \leq 2 \exp \left( - \frac{C_1 t^2}{2 \|A\|_F^2 \|\mu\|^2} \right). \tag{3.13} \]

Therefore by Lemma 3.3,

\[ P'(\|e^T A \mu\| \geq t) \leq 2 \exp \left( - \frac{C_1 n t^2}{\gamma_d \|\mu\|^2} \right). \]

For any \(C_2 > 0\), Markov’s inequality gives

\[ \mathbb{P}(\|\mu\|^2 > C_2 n) \leq \mathbb{E}(e^{|\mu|^2 / K_2}) \exp \left( - \frac{C_2 n}{K_2} \right) \leq 2^n \exp \left( - \frac{C_2 n}{K_2} \right). \]

Therefore this gives us

\[ \mathbb{P}(\|e^T A \mu\| \geq t) \leq 2 \mathbb{E} \left[ \exp \left( - \frac{n^2 t^2}{\gamma_d \|\mu\|^2} \right) \right] \leq 2 \exp \left( - \frac{n C_1 t^2}{C_2 \gamma_d} \right) + 2 \mathbb{E} \left[ \exp \left( - \frac{n^2 t^2}{\gamma_d \|\mu\|^2} \right) \right] \mathbb{1}\{\|\mu\|^2 > n C_2 \} \leq 2 \exp \left( - \frac{n C_1 t^2}{C_2 \gamma_d} \right) + 2 \exp \left( n \left( \log 2 - \frac{C_2}{K_2} \right) \right). \tag{3.14} \]

Combining (3.10) and (3.14), we get

\[ \mathbb{P}(|f(k) - g(k)| \geq t) \leq 2 \exp \left( - n \min \left\{ \frac{t^2}{K_1^2 \gamma_d}, \frac{t}{K_1 \gamma_d} \right\} \right) + 2 \exp \left( - \frac{n C_1 t^2}{C_2 \gamma_d} \right) + 2 \exp \left( n \left( \log 2 - \frac{C_2}{K_2} \right) \right). \]

The proof is completed by choosing \(C_2\) such that \(\log 2 - C_2 / K_2 = -1\). \(\square\)

of Lemma 3.2. Let \(b_i\) be the \(i\)-th row of matrix \(B\). Then

\[ \|A\|^2_F = \frac{1}{n^2} \sum_{i,j} (b_i, b_j)^2 \]

\[ = \frac{1}{n} \left( 1 + \frac{1}{K} \right) + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j \neq i} (b_i, b_j)^2. \]
For any distinct $i, j$,
\[
\langle b_i, b_j \rangle = -\frac{1}{k} \{i \in N_k(j)\} + 1_{\{j \in N_k(i)\}} + \frac{1}{k^2} |N_k(i) \cap N_k(j)|,
\]
and therefore
\[
|\langle b_i, b_j \rangle| \leq \frac{2}{k}. \tag{3.15}
\]
This show that for any $i$,
\[
\sum_{j \neq i} \langle b_i, b_j \rangle^2 \leq \frac{4}{k^2} \{ j : \langle b_i, b_j \rangle \neq 0 \}. \tag{3.16}
\]
But if $\langle b_i, b_j \rangle \neq 0$, then
\[
\left( \{i\} \cup N_k(i) \right) \cap \left( \{j\} \cup N_k(j) \right) \neq \emptyset. \tag{3.17}
\]
By definition $|N_k(i)| = k$, and for any $\ell$, by [17, Corollary 6.1] there are at most $\gamma d k$ indices $j$ such that $\ell \in N_k(j)$. Therefore for any $i$,
\[
|\{ j : \langle b_i, b_j \rangle \neq 0 \}| \leq \gamma d k (k + 1). \tag{3.18}
\]
This gives the required bound on $\|A\|_F^2$. \hfill \Box

**of Lemma 3.3.** Take any $x$ such that $\|x\| = 1$. Then by [17, Corollary 6.1],
\[
\|Bx\|^2 = \sum_{i=1}^{n} \langle b_i, x \rangle^2 \\
\leq 2 \sum_{i=1}^{n} x_i^2 + 2 \sum_{i=1}^{n} \left( \frac{1}{k} \sum_{j \in N_k(i)} x_j \right)^2 \\
\leq 2\|x\|^2 + 2 \sum_{i=1}^{n} \sum_{j \in N_k(i)} x_j^2 \\
= 2\|x\|^2 + 2 \sum_{j=1}^{n} \sum_{i:j \in N_k(i)} x_j^2 \\
\leq \gamma d \|x\|^2.
\]
Therefore $\|B\|_2 \leq \gamma d$ and hence $\|A\|_2 \leq \gamma d/n$. \hfill \Box

An R language package **knnopt** will soon be made available on the CRAN repository.

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