Convergence of Nearest Neighbor Pattern Classification with Selective Sampling

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1 Introduction

In the panoply of pattern classification techniques, few enjoy the intuitive appeal and simplicity of the nearest neighbor rule: given a set of samples in some domain space whose value under some function is known, estimate the function anywhere in the domain by giving the value of the nearest sample (relative to some metric). More generally, one may use the modal value of the $m$ nearest samples, where $m \geq 1$ is some fixed integer constant, although $m = 1$ is known to be admissible in the sense that there is no $m > 1$ that is asymptotically superior in terms of prediction error [2].

The nearest neighbor rule is a nonparametric technique; that is, it does not make any assumptions about the character of the underlying function (eg, linearity) and proceed to estimate parameters modulo this assumption (eg, slope and intercept). Furthermore, it is extremely general, requiring in principle only that the domain be a metric space.

The classic paper on nearest neighbor pattern classification is due to Cover and Hart [2]; a textbook treatment appears in Duda et al. [4]. Both presentations adopt a probabilistic setting, demonstrating that if the samples are independent and identically-distributed (iid), the probability of error converges to no more than twice the optimal probability of error, the so-called Bayes risk. In a fully deterministic setting, since the Bayes risk is zero, this amounts to showing that the nearest neighbor rule with iid sampling converges to the true pattern. Cover [1] extends these results to the estimation problem.

Obviously iid sampling is almost certain to produce samples that are superfluous in the sense that the prediction remains equally accurate even if these samples are removed.

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Superfluous samples are harmful in two senses: first, sampling may be—and usually is—difficult in one way or another; second, it is computationally more expensive to search for a point’s nearest neighbor as the size of the sample set increases.

The latter concern can be addressed by editing techniques, in which a large set of pre-classified samples is shorn down by deleting samples according to some rule. Wilson [12] shows that convergence holds when one deletes samples that are misclassified by their \( m \geq 2 \) nearest neighbors, and then uses the nearest neighbor rule on the remaining samples. (Wagner [11] simplifies the proof considerably.) An conceptually simpler algorithm involving Voronoi diagrams is given in [4], but this is unlikely to be practical for reasons described in §3.2.2.

Of course editing can only delete samples already taken and cannot address the desire to sample parsimoniously in the first place. This is achieved by selective sampling, wherein each sample is selected from a pool of candidates according to some heuristic function. The trick lies in identifying some heuristic such that the odds of choosing a superfluous (or otherwise “low-information”) sample are reduced. Selective sampling falls within the broader paradigm of active learning, which is surveyed by Settles [8].

Fujii et al. [5] present a nearest neighbor algorithm for word sense disambiguation using selective sampling. The problem is interesting because the domain space is non-Euclidean, but the selection heuristic is quite specific to problems in natural language. Lindenbaum et al. [7] give a more general treatment, including very abstract descriptions of the selection heuristic. However, they assume that the domain is Euclidean and that the true pattern conforms to a particular random field model. The selection heuristic is also complex and computationally expensive.

This paper seeks to take the intuition of selective sampling back to the extremely general setting of [2], assuming not much more than a metric domain on which exists a probability measure. We will give three selection heuristics and prove that their nearest neighbor rule predictions converge to the true pattern; furthermore, the first and third of these algorithms are computationally cheap, with complexity growing only linearly in the number of samples in the naive implementation. We believe that proving convergence in such a general setting with such simple algorithms constitutes an important advance in the art.

Following the present introductory section, in §2 we establish the problem’s formal setting. §3 contains the key convergence proofs, plus additional results and remarks relating to the practical use of the methods. We conclude the paper and indicate avenues for future research, including the crucial question of convergence rates, in §4.

### 2 Preliminaries

In this section we lay down some common definitions and notation that we will use throughout the rest of the paper. The object of our efforts will be to approximate a classifier function \( f : X \to Y \), the so-called true function, where the domain \( X \) is a metric space equipped with

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1Settles uses the term pool-based sampling, but selective sampling seems to be the term of art among researchers using nearest neighbor techniques.
metric $d$ and probability measure $\mu$; and the codomain $Y$ is any countable set. We approximate $f$ using a sequence of samples $\{z_n\}_{n=1}^{\infty}$ from $X$ collected into sets $Z_n = \{z_1, z_2, \ldots, z_n\}$. The prediction function $\zeta_n : X \to Y$ operates via the nearest neighbor rule on $Z_n$; that is:

$$\zeta_n(x) = f(z_\iota) \text{ where } \iota = \arg\min_{i \leq n} d(x, z_i).$$  

(1)

(If more than one sample achieves the minimum distance to $x$, choose one uniformly at random.)

It should be noted that in contrast to the works cited in \S1, the true function is fully determined, not probabilistic. We have chosen a deterministic setting for two reasons. In the first place, we confess, it makes the analysis much easier. More fundamentally, however, the algorithms we develop in \S3.2 break with the concept that the nearest sample to any point approaches arbitrarily near to the point, which is a critical assumption underlying the calculation of prediction error in terms of Bayes risk. Recovering the probabilistic setting is an area of future research and discussed in \S4.

Given a point $x \in X$, the (open) $\epsilon$-ball about $x$, denoted $B_\epsilon(x)$, is the set of points at distance strictly less than $\epsilon$ from $x$. The support of $\mu$, or supp($\mu$), are the points of $x \in X$ such that the $\epsilon$-ball about $x$ has positive measure for all $\epsilon > 0$.

We will be concerned with two types of convergence. Let $\{f_n\}_{n=1}^{\infty}$ be a sequence of functions. Given $S \subseteq X$, the sequence converges pointwise to $f$ on $S$ iff

$$\forall s \in S : \lim_{n \to \infty} f_n(s) = f(s).$$

We also write: $f_n \to f$ pointwise on $S$; or for any particular $s \in S$: $f_n(s) \to f(s)$. Furthermore, the sequence of functions converges in measure to $f$ iff it converges pointwise to $f$ on all of $X$ save for a set of measure zero. We write this more briefly as: $f_n \to f$ in measure.

When we say an event occurs almost surely, almost certainly, or suchlike, we mean that it occurs with probability one with respect to the probability measure $\mu$; the phrases almost never, almost impossible, and so forth, are attached to an event with probability zero. In this work, these terms will typically be associated with invocations and implications of the following classical lemma in probability theory.

**Second Borel-Cantelli Lemma.** Let $\{E_n\}_{n=1}^{\infty}$ be a sequence of independent events in some probability space. If

$$\sum_{n=1}^{\infty} \Pr[E_n] = \infty$$

then

$$\Pr[\lim\sup E_n] = 1.$$  

In other words, almost surely $E_n$ occurs for infinitely many $n$.

Our goal is to show that $\zeta_n \to f$ pointwise on supp($\mu$) almost surely under certain instantiations of the following stochastic process:
1. \( n \leftarrow 1 \).

2. Select at random (per \( \mu \)) a \( \kappa(n) \)-set \( S \subseteq X \) of candidates.

3. \( z_n \leftarrow \arg \max_{s \in S} \Phi(s, Z_{n-1}) \). (If there is more than one candidate that achieves the maximum, choose one uniformly at random.)

4. \( n \leftarrow n + 1 \).

5. Go to Step 2.

We call this process \( S(\kappa, \Phi) \): it is parameterized by a function \( \kappa : \mathbb{Z}^+ \rightarrow \mathbb{Z}^+ \) that determines the number of candidates; and a selection heuristic \( \Phi : X \times \mathcal{P}(X) \rightarrow \mathbb{R} \) that somehow expresses how “desirable” a candidate would be as a sample, given the preceding samples.\(^2\)

Finally, if \( X \) is separable—that is, if it contains a countable dense subset—then we will show that in fact \( \zeta_n \rightarrow f \) in measure as an immediate corollary of the corresponding pointwise convergence result.

### 2.1 Selective sampling may fail badly

Before starting in earnest, it may be valuable to understand how an arbitrary sequence of samples may fail to converge to \( f \). Indeed, we shall give an example such that the prediction functions \( \zeta_n \) have monotonically decreasing accuracy. Although our example will be rather contrived, it will show that some care must be taken when designing the sampling process.

Let \( X = [0, 1] \subset \mathbb{R} \) with Euclidean metric \( d \) and Lebesgue measure \( \mu \); and let \( Y = \{0, 1\} \). Now let

\[
X_1 = \{0\} \cup \bigcup_{i=1}^{\infty} \left( \frac{1}{2^i} \cdot \frac{3}{2^i + 1} + \epsilon_i \right) \quad \text{where} \quad 0 < \epsilon_i < \frac{1}{2^{i+1}}
\]

and take \( f \) to be the indicator function on \( X_1 \).

Suppose we take samples according to the process \( z_1 = 0 \) and \( z_n = 2^{-n} \) for \( n \geq 2 \). Observe that for each \( \zeta_n \) where \( n \geq 2 \), we are newly accurate on a set of measure less than \( \epsilon_{n-1} \), but newly inaccurate on a set of measure greater than \( 2^{-n} \); and since \( \epsilon_{n-1} < 2^{-n} \) by definition, we become less accurate with each increment of \( n \).

It should also be observed that the sample sequence corresponds to an intuitively very reasonable selection method: \( z_n \) is the midpoint of two samples with different \( f \)-values (for all \( n \geq 3 \)).

### 3 Selective sampling heuristics

We consider two choices for the selection heuristic \( \Phi \): distance to sample set and (two variants of) non-modal count. Of the two, non-modal count is certainly the more interesting and useful; the distance to sample set heuristic mostly mimics the action of iid sampling,

\(^2\)In \[5, 7\] the selection heuristic is called the utility function, but we prefer the more elastic term.
although it turns out to be a useful way to present some basic ideas that will be used again in more complicated settings.

Let us articulate some definitions that connect $f$ with the geometry and measure of $X$. For any $y \in Y$, let $X_y = f^{-1}(y) = \{x \in X: f(x) = y\}$. A subset $R \subseteq X$ is called $f$-connected iff $R$ is connected and there exists $y \in Y$ such that $R \subseteq X_y$. An $f$-connected set that is maximal by inclusion in $X$ is an $f$-connected component. Consider a point $b \in X$ on the boundary of an $f$-connected component: we say $b$ is an $f$-boundary point iff $f(b) = y$ yet $\mu(B_\epsilon(b) \cap (X - X_y)) > 0$ for all $\epsilon > 0$. The $f$-boundary is simply the set of all $f$-boundary points.

As a general rule, we only consider points off the $f$-boundary. This assumption is necessary for the nearest neighbor rule to be valid, since any $f$-boundary point can have a “misleading” sample arbitrarily close to it. In order to free ourselves of the burden of the $f$-boundary, we typically assume that it has measure zero—which is generally a very natural assumption, provided that $Y$ is countable.

### 3.1 Distance to sample set

The distance to sample set heuristic $\Phi$ is defined very simply as:

$$\Phi(x, S) = d(x, S) = \inf\{d(x, s); s \in S\}. \tag{2}$$

This leads to our first convergence theorem.

**Theorem 1.** Let $\{z_n\}_{n=1}^\infty$ be determined by the process $S(\kappa, \Phi)$ where $\kappa : \mathbb{Z}^+ \to \mathbb{Z}^+$ is such that, for any $0 < \rho \leq 1$,

$$\sum_{n=1}^\infty \rho^{\kappa(n)} = \infty$$

and $\Phi$ is defined by (2). If $x \in \text{supp}(\mu)$ is not an $f$-boundary point, then $\xi_n(x) \to f(x)$ with probability one.

**Proof.** Let $Q_n^r \subseteq X$ denote the points $q$ such that $\Phi(q, Z_n) \geq \epsilon$, and let $Q^\epsilon = \limsup Q_n^\epsilon$ (ie, $q \in Q_\epsilon$ iff $q$ appears in infinitely many $Q_n^\epsilon$). For any point $x \in \text{supp}(\mu)$ that is not an $f$-boundary point, there exists $r > 0$ such that $\mu(B_r(x) - X_{f(x)}) = 0$; we fix some such point $x$ and distance $r$.

Denote by $E_n$ the event that one of the $\kappa(n+1)$ candidates for $z_{n+1}$ lies in $B_{r/2}(x)$, while all the others lie in $X - Q_{n+1}^{r/2}$. Hence

$$\Pr[E_n] = \kappa(n+1)\mu(B_{r/2}(x))(1 - \mu(Q_{n+1}^{r/2}))^{\kappa(n+1)-1}.$$ 

Observe that $\mu(B_{r/2}(x))$ is positive (since $x \in \text{supp}(\mu)$) and constant with respect to $n$. $\mu(Q_{n+1}^{r/2})$ does vary with $n$, of course, but $Q_{n+1}^{r/2} \subseteq Q_n^{r/2}$, so the measure is nonincreasing in $n$. Therefore the quantity $(1 - \mu(Q_n^{r/2}))$ can be bounded below by some $0 < \rho \leq 1$ for large $n$ (almost always)\(^3\)

\(^3\)The case that $\mu(Q_n^{r/2}) = 1$ for large $n$ occurs with probability zero since it requires that all relevant $Z_n$ lie entirely outside $\text{supp}(\mu)$, which can be excluded by the First Borel-Cantelli Lemma.
Suppose $\kappa(n) \leq k$ for infinitely many $n$; then for these $n$,

$$\Pr[E_n] \geq \mu(B_{r/2}(q))\rho^{k-1}.$$ 

Since the right-hand side is a constant greater than zero, the sum of the $\Pr[E_n]$ must diverge to infinity. On the other hand, if the sequence of $\kappa(n)$ has no bounded subsequence, then for sufficiently large $n$, $\kappa(n) \geq \mu(B_{r/2}(q))^{-1}$. Thus

$$\Pr[E_n] \geq (1 - \mu(Q_n^{r/2}))^{\kappa(n+1)-1} \geq \rho^{\kappa(n+1)}$$

for large $n$; it follows that $\sum_{n=1}^{\infty} \Pr[E_n] = \infty$. So in either case the Second Borel-Cantelli Lemma tells us that $E_n$ occurs infinitely often with probability one.

In the event $E_n$, let $q$ denote the candidate in $B_{r/2}(x)$. If $q \notin Q_n^{r/2}$, then there exists $i \leq n$ such that $z_i \in B_{r/2}(q)$—but since $B_{r/2}(q) \subseteq B_r(x)$, this contradicts $x \in Q^r$. Hence $q \in Q_n^{r/2}$, so it will be chosen as $z_{n+1}$, since all other candidates will have smaller $\Phi$-values. Consequently, $x \notin Q^r$ for any $i \geq 1$—which also contradicts $x \in Q^r$.

Thus $x \notin Q^r$, meaning that a sample is eventually placed less than distance $r$ from $x$. Such a sample would have the same $f$-value as $x$ with probability one, and we conclude that $\zeta_n(x) \rightarrow f(x)$ almost always.

**Remark 1.** Given any $x \in \text{supp}(\mu)$, one can use the following “brute force” argument to prove that a sample will eventually be placed arbitrarily close to $x$: for any $\epsilon > 0$, $\mu(B_{\epsilon}(x)) > 0$, so all of the $\kappa(n+1)$ candidates for $z_{n+1}$ will lie in $B_{\epsilon}(x)$ infinitely often because

$$\sum_{n=1}^{\infty} \mu(B_{\epsilon}(x))^{\kappa(n+1)} = \infty.$$ 

This argument, while a formally correct use of the Second Borel-Cantelli Lemma, is sterile in substance since it does not suggest why selective sampling has any advantage over iid sampling; indeed, it suggests that iid sampling (ie, $\kappa(n) = 1$) is superior. Our proof, on the other hand, demonstrates that it suffices for one candidate to appear near $x$, provided that all others lie in regions with lower $\Phi$-values.

A key theme of this paper will be avoiding “brute force” arguments; or, when they seem to be unavoidable, demonstrating how to mitigate their impact.

**Remark 2.** It is not difficult to see that $\kappa$ is admissible if $\kappa(n) \leq k$ infinitely often for some constant $k$. It is also possible that $\kappa(n) \rightarrow \infty$, provided that it grows very slowly; consider, for example,

$$\kappa(n) \leq H_{\lfloor \lg(n+1) \rfloor} = \sum_{i=1}^{\lfloor \lg(n+1) \rfloor} \frac{1}{i}.$$ 

This can be proven admissible by means of the Cauchy Condensation Test. The practical value in selecting an unbounded $\kappa$ is to help “find” the subsets of $X$ with high $\Phi$-values, since the measure of such subsets decreases as $n \rightarrow \infty$.

Cover and Hart establish the following lemma in [2].
Lemma 2 (Cover and Hart [2]). Suppose $X$ is a separable metric space, and let $S \subseteq X$. If $S \cap \text{supp}(\mu) = \emptyset$, then $\mu(S) = 0$.

With Lemma 2, convergence in measure flows immediately from Theorem 1.

**Corollary.** Suppose $S(\kappa, \Phi)$ is as described by Theorem 1. If $X$ is separable, and the $f$-boundary has measure zero, then $\zeta_n \rightarrow f$ in measure with probability one.

**Proof.** If $x \in \text{supp}(\mu)$ is not an $f$-boundary point, then $\zeta_n(x) \rightarrow f(x)$ almost surely by Theorem 1. Hence any point that does not converge to its $f$-value is either an $f$-boundary point or outside $\text{supp}(\mu)$—but since the $f$-boundary has measure zero by assumption, and $\mu(X - \text{supp}(\mu)) = 0$ by Lemma 2 the set of all such points has measure zero.

### 3.2 Non-modal count

The distance to sample set heuristic produces samples that tend to “spread out” over $X$ geometrically (unlike iid sampling, which is sensitive only to $\mu$). If one’s goal is to approximate the true function $f$, however, this is still not the most efficient arrangement of samples: what one really wants to do is place “very many” samples near the $f$-boundary and “very few” samples elsewhere.

Predictions under the nearest neighbor rule are naturally visualized as *Voronoi diagrams* (also known as *Voronoi tessellations*, *Voronoi decompositions*, or *Dirichlet tessellations*) that partition $X$ according to its nearest neighbor in $Z_n$; see, for instance, §4 of Devadoss and O’Rourke [3]. We motivate the point in the preceding paragraph by examining Voronoi diagram predictions of the “bat insignia” [13] under different sampling methods. For this example, $X$ is a subset of the Euclidean plane; $Y = \{0, 1\}$; and $\mu$ is the uniform distribution.

In Figure 1, the diagrams are constructed over sets of iid samples; note that the cells are roughly the same size in each diagram, exactly as one would expect with iid samples. Figure 2 on the other hand, shows diagrams constructed with a selective sampling method; here we observe that the cells are very small near the $f$-boundary and large elsewhere.
Comparing each diagram in Figure 1 with its correspondent in Figure 2, clearly the latter achieves a more accurate prediction with (virtually) the same number of samples.

The non-modal count heuristic $\Phi$ is defined as:

$$\Phi(x, S) = |V_S(x)| - \text{modefreq}_f(V_S(x))$$

where $V_s : X \to \mathcal{P}(S)$ maps $x$ to some (possibly empty) set of neighbors in $S$; and $\text{modefreq}_f(A)$ denotes the frequency of the mode of $A$ under $f$. Below we give two alternatives for $V_S$ and prove convergence for both.

### 3.2.1 Voronoi neighbors

We have already observed that Voronoi diagrams are the natural visualization of the nearest neighbor rule, so it is natural to expect that their formal properties might be useful. As it turns out, we will not require very much from the theory of Voronoi diagrams, save the following definition: given $x \in X$ and $S \subseteq X$, we say that $v \in S$ is a Voronoi neighbor of $x$ if there exists a point $c \in X$ for which $d(x, c) < d(v, c) \leq d(s, c)$ for any $s \in S$. With reference to (3) above, then, we can define $V_S(x)$ as the set of all Voronoi neighbors of $x$ with respect to $S$.

Stated another way, $v$ is a Voronoi neighbor of $x$ if there is some point in $X$ (ie, $c$) whose nearest neighbor in $S$ is $v$, yet whose nearest neighbor in $S \cup \{x\}$ is $x$. (Observe that $V_S(x) = \emptyset$ iff $x \notin S$. Furthermore, if $x \notin S$, then its nearest neighbor in $S$ is always a Voronoi neighbor: let $c = x$.) This definition is well-suited to analyze the evolution of predictions: if a candidate with positive non-modal count is selected as a sample, the prediction function changes, since at least one point will be predicted differently.

The following lemma, which shows that Voronoi neighbors are preserved in sufficiently small neighborhoods, will be helpful in our investigations.
Lemma 3. Let $S \subseteq X$. For any $x \in X - S$, if $v \in V_S(x)$, then there exists $\epsilon > 0$ such that for all $x' \in B_\epsilon(x)$, $v \in V_S(x')$. Furthermore, if $v$ is the nearest neighbor of $x$ in $S$, then the previous statement holds for all $0 < \epsilon \leq d(x, v)$.

Proof. By definition there exists $c \in X$ such that $d(x, c) < d(v, c) \leq d(s, c)$ for any $s \in S$. Let $0 < \epsilon \leq d(v, c) - d(x, c)$. By the triangle inequality, for any $x' \in B_\epsilon(x)$ we have

$$d(x', c) \leq d(x', x) + d(x, c) < \epsilon + d(x, c) \leq d(v, c)$$

so $v \in V_S(x')$. The final claim is established by letting $c = x$. \hfill \square

Before proceeding to our next convergence result, we will require two more definitions. An $f$-connected set $R$ is said to be $f$-contiguous iff $R$ is a subset of supp($\mu$) and does not contain $f$-boundary points. A maximal $f$-contiguous set is an $f$-contiguous component.

Theorem 4. Let $\{z_n\}_{n=1}^\infty$ be determined by the process $S(\kappa, \Phi)$ where $\kappa$ is such that, for any $0 < \rho \leq 1$,

$$\sum_{n=1}^\infty \rho^{\kappa(n)} = \infty$$

and $\Phi$ is defined by (3), with $V_S(x)$ denoting the Voronoi neighbors of $x$ with respect to $S$. If $x \in X$ is contained in an $f$-contiguous component of positive measure, then $\zeta_n(x) \to f(x)$ with probability one.

Proof. Let $W_n \subseteq X$ be the set of points $w$ such that $\zeta_n(w) \neq f(w)$; and let $W = \limsup W_n$. We wish to show that no point contained in an $f$-contiguous component of positive measure is also contained in $W$. Suppose, for the sake of contradiction, that such a point $x$ exists.

Let $C$ denote the $f$-contiguous component containing $x$. We claim that a sample will eventually be placed in $C$ almost surely. By assumption, $\mu(C) > 0$. Let $G_n$ be the event that all of the $\kappa(n + 1)$ candidates for $z_{n+1}$ lie in $C$; then

$$\sum_{n=1}^\infty \Pr[G_n] = \sum_{n=1}^\infty \mu(C)^{\kappa(n+1)} = \infty$$

and the Second Borel-Cantelli Lemma tell us that $G_n$ occurs infinitely often. The claim follows immediately; but see Remark 3.

Every metric space has a unique (up to isometry) completion, so let $\bar{X}$ denote the completion of $X$. We can extend $f$ to every point in $\bar{X}$ in the following way: for any $\bar{x} \in \bar{X} - X$, if there exists $y \in Y$ and $\epsilon > 0$ such that $B_\epsilon(\bar{x}) \cap X \subseteq X_y$, then $f(\bar{x}) = y$; otherwise $f(\bar{x})$ may be assigned any value in $Y$. We also extend $\mu$ to $\bar{X}$ by letting $\mu(\bar{X} - X) = 0$. In this way we allow ourselves to work in $X$ or $\bar{X}$ interchangeably.

Consider $\partial W \subseteq \bar{X}$, the boundary of $W$. We say that $\partial W$ crosses $C$ at $b$ iff $b \in \partial W$ is not an $f$-boundary point and $B_\epsilon(b)$ has nonempty intersection with both $C \cap W$ and $C - W$ for all $\epsilon > 0$. If $\partial W$ does not cross $C$ at any point, then $x \in C$ implies $C \subseteq W$, which is inconsistent with a sample being placed in $C$; thus $\partial W$ almost certainly crosses $C$. 

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Let $b$ denote a point at which $\partial W$ crosses $C$; since it is not an $f$-boundary point, there exists $r > 0$ such that $\mu(B_r(b) - X_{f(b)}) = 0$. From this it follows that $d(b, z_n) \geq r$ for all $n$ almost surely. Now for any $0 < \alpha < r$, we can find $b_1, b_2 \in B_{\alpha}(b)$ such that $b_1 \notin W$ and $b_2 \in W$. Hence for infinitely many $n$, Lemma 3 implies that any point in $B_{r-\alpha}(b_1)$ has a Voronoi neighbor in $Z_n$ with the same $f$-value as $b$; and similarly that any point in $B_{r-\alpha}(b_2)$ has a Voronoi neighbor in $Z_n$ with $f$-value different from $b$. Taking $\alpha$ sufficiently small allows us to choose $0 < \epsilon < r$ such that

$$B_{\epsilon}(b) \subset B_{r-\alpha}(b_1) \cap B_{r-\alpha}(b_2).$$

Let $Q_n \subset X$ denote the points $q$ such that $\Phi(q, Z_n) > 0$, and let $Q = \lim \sup Q_n$. Because every point in $B_{\epsilon}(b)$ has (at least) two Voronoi neighbors with different $f$-values in infinitely many $Z_n$ (almost surely), there is an infinite subsequence $\{n_i\}_{i=1}^\infty$ such that $B_{\epsilon}(b) \cap X \subseteq Q_{n_i}$; so in fact, $B_{\epsilon}(b) \cap X \subseteq Q$ (with probability one).

By the definition of $b$, there exists $c \in B_{\epsilon}(b) \cap C \cap W$. Since $c \in C$ means that $c$ is not an $f$-boundary point, there exists $\gamma_1 > 0$ such that $\mu(B_{\gamma_1}(c) - X_{f(c)}) = 0$; furthermore, there exists $\gamma_2 > 0$ such that $B_{\gamma_2}(c) \subseteq B_{\epsilon}(b)$. Set $\gamma = \min(\gamma_1, \gamma_2)$, and note that $\gamma$ is constant with respect to $n_i$. Let $E_i$ denote the event that one of the $\kappa(n_i + 1)$ candidates for $z_{n_i + 1}$ lies in $B_{\gamma}(c)$ while all others lie in $X - Q_{n_i}$. Thus

$$\Pr[E_i] = \kappa(n_i + 1)\mu(B_{\gamma}(c))(1 - \mu(Q_{n_i}))^{\kappa(n_i + 1) - 1}.$$

Since $c \in C \subseteq \text{supp}(\mu)$, $\mu(B_{\gamma}(c)) > 0$.

Now for $i$ sufficiently large, $\mu(Q_{n_i})$ is arbitrarily close to $\mu(Q)$. If $\mu(Q) < 1$, then $1 - \mu(Q_{n_i})$ is bounded away from zero; we can then employ the same argument as in the proof of Theorem 1 to show that $E_i$ occurs infinitely often with probability one. In the event $E_i$, since the candidate in $B_{\gamma}(c)$ is the only one with positive non-modal count, we will have $z_{n_i + 1} \in B_{\gamma}(c) \subseteq B_{\gamma_1}(c)$, which implies that $c \notin W$ almost surely.

If, on the other hand, $\mu(Q) = 1$, we resort to the “brute force” event $F_n$ in which all candidates lie in $B_{\gamma}(c)$. (However, see Remark 4.) Now

$$\sum_{n=1}^\infty \Pr[F_n] = \sum_{n=1}^\infty \mu(B_{\gamma_1}(c))^{\kappa(n+1)} = \infty,$$

so the Second Borel-Cantelli Lemma says that $F_n$ occurs infinitely often with probability one. But if $F_n$ occurs, $c \notin W$ almost surely.

We have, at last, obtained a contradiction. We conclude that if $x$ is contained in an $f$-contiguous component of positive measure, then almost surely $x \notin W$; in other words, $\zeta_n(x) \to f(x)$ with probability one. \qed

An important aspect of the proof is that, although we ultimately derive at contradiction at the point $x$, this is effected by placing points close to $c$, a point in the same $f$-contiguous component as $x$, but otherwise not assumed to be close to $x$. This means that relatively sparse sampling in the “middle” of $f$-contiguous components suffices, as suggested by Figure 2.
Corollary. Suppose $\mathcal{S}(\kappa, \Phi)$ is as described by Theorem 4. If $X$ is separable; the $f$-boundary has measure zero; and the union of all $f$-contiguous components with measure zero itself has measure zero; then $\zeta_n \to f$ in measure with probability one.

Remark 3. If an $f$-contiguous component does not contain at least one sample, it is possible for it to be “overlooked” by the non-modal count heuristic. A “brute force” invocation of the Second Borel-Cantelli Lemma is therefore used to show that a sample is eventually placed in every $f$-contiguous component of positive measure. In practice, however, one would prefer to have samples placed in every such component through some a priori process. For example, if it is known that every $f$-contiguous component (about which one cares) has measure at least $p$, placing $\max(20, 5/p)$ initial iid samples gets a sample in each component with over 99 percent confidence (as a consequence of the Central Limit Theorem).

Remark 4. If $Q$, the set of points with non-modal counts that never settle to zero, has measure equal (or close) to one, the proof has a “brute force” aspect that we claimed to avoid in Remark 1. Some reflection on the problem will show that $X$ has to be somewhat “weird” for such $Q$ to occur, because we generally expect the Voronoi neighbors close to some point to “block out” any potential neighbors far from the point. Proposition 5 makes this insight precise by showing that, in fact, $\mu(Q) = 0$ under certain reasonable conditions.

Recall that a metric space with metric $d$ is a length space iff for any points $x, y$ in the space, $d_I(x, y) = d(x, y)$, where $d_I$ is the infimum of the lengths of all paths from $x$ to $y$.

Proposition 5. Suppose $\mathcal{S}(\kappa, \Phi)$ is as described by Theorem 4 and assume that all the following obtain:

1. $X$ is separable;
2. the completion of $X$ is a length space; and
3. for every $x \in \text{supp}(\mu)$ that is not an $f$-boundary point, there exists $\omega > 0$ such that $B_\omega(x) \subseteq \text{supp}(\mu)$.

Let $Q_n = \{x \in X; \Phi(x, Z_n) > 0\}$. If the $f$-boundary has measure zero, then $\mu(\limsup Q_n) = 0$ with probability one.

Proof. Let $Q = \limsup Q_n$. Suppose, for the sake of contradiction, that there exists $q \in Q \cap \text{supp}(\mu)$ off the $f$-boundary. There exists $r > 0$ such that $\mu(B_r(q) - X_f(q)) = 0$; set $\epsilon = \min(r, \omega)$, where $\omega$ is as defined above. Note that $\epsilon$ does not depend on $n$.

Let $\bar{X}$ denote the completion of $X$; we can use $X$ and $\bar{X}$ interchangeably by the same techniques used in the proof of Theorem 4. Let $S_\gamma(q) \subseteq \bar{X}$ denote the boundary of the $\gamma$-ball about $q$. Consider $S_{\epsilon/2}(q)$: this set can obviously be covered by a finite set of $\epsilon/4$-balls about some points $x_1, x_2, \ldots, x_m \in S_{\epsilon/2}(q)$.

Let $E_{i,n}$ be the event that one of the $\kappa(n + 1)$ candidates for $z_{n+1}$ lies in $B_{\epsilon/4}(x_i)$ while all others lie in the set

$$L_{i,n} = B_{\epsilon/4}(x_i) \cup \{l \in Q_n; \forall x \in B_{\epsilon/4}(x_i) : \Phi(l, Z_n) < \Phi(x, Z_n)\}.$$
Thus

$$\Pr[E_{i,n}] = \kappa(n+1)\mu(B_{\epsilon/4}(x_i))\mu(L_{i,n})^{\kappa(n+1)-1} \geq \mu(B_{\epsilon/4}(x_i))^{\kappa(n+1)}.$$ 

Because $x_i$ is a limit point, there exists $x'_i \in X$ arbitrarily close to $x_i$; thus some sufficiently small ball about $x'_i$ will be contained in $B_{\epsilon/4}(x_i)$. Furthermore, since

$$x'_i \in B_{\epsilon}(q) \subseteq B_{\omega}(q) \subseteq \text{supp}(\mu)$$

it must be that $\mu(B_{\epsilon/4}(x_i)) > 0$ and $\Pr[E_{i,n}]$ is bounded away from zero. So the sum of the $\Pr[E_{i,n}]$ diverges to infinity, and by the Second Borel-Cantelli Lemma, $E_{i,n}$ occurs infinitely often with probability one. Now in the event $E_{i,n}$, a candidate in $B_{\epsilon/4}(x_i)$ will become $z_{n+1}$.

We conclude that for $n$ sufficiently large, almost certainly $Z_n$ has at least one element in every $B_{\epsilon/4}(x_i)$ where $1 \leq i \leq m$.

Since $q \in Q$, there exist arbitrarily large $n$ such that $q \in Q_n$. For such $n$, $q$ has a Voronoi neighbor $z_a \in Z_n$ such that $f(z_a) \neq f(q)$; so almost surely $d(z_a, q) \geq r$, given that $q$ is not an $f$-boundary point. Let $c$ be a point that certifies that $z_a \in V_{Z_n}(q)$.

Suppose $c \notin B_{\epsilon/2}(q)$. Now for any $\delta > 0$, there exists $c' \in S_{\epsilon/2}(q)$ with

$$d(q, c') + d(c', c) < d(q, c) + \delta.$$ 

This is a consequence of the fact that $X$ is a length space: one can think of $c'$ as the point where an almost-shortest path from $q$ to $c$ intersects $S_{\epsilon/2}(q)$. But for large $n$, as there is a sample in every $B_{\epsilon/4}(x_i)$, there will almost surely be $z_b \in Z_n$ such that $d(z_b, c') < \epsilon/2 = d(q, c')$. So:

$$d(z_b, c) \leq d(z_b, c') + d(c', c) < d(q, c') + d(c', c) < d(q, c) + \delta.$$ 

Yet since $\delta$ may be arbitrarily small, in fact $d(z_b, c) < d(q, c)$. This contradicts the character of $c$.

Alternatively, suppose $c \in B_{\epsilon/2}(q)$; we take $c'$ as before, except this time on a path from $z_a$ to $c$. With $z_b$ as before, $d(z_b, c') < \epsilon/2 \leq r/2 \leq d(z_a, c')$. Reasoning exactly as above, $d(z_b, c) < d(z_a, c')$—which is also a contradiction.

Both alternatives being contradictory, we conclude that $q \notin Q$; so in fact, $Q$ is disjoint from $\text{supp}(\mu)$, save for the $f$-boundary. As $X$ is separable, Lemma 2 applies, and given that the $f$-boundary has measure zero, we conclude that $\mu(Q) = 0$. 

Observe that Proposition 3 is satisfied for a Euclidean space; or indeed for the space of rational points of any dimension, since its completion is Euclidean.

### 3.2.2 $K$-nearest neighbors

Reasoning in terms of Voronoi neighbors is desirable since it closely reflects the evolution of the Voronoi diagrams $\zeta_n$; however, calculation of the Voronoi neighbors is typically difficult. The definition given above is unsuitable for computation, since it does not suggest any method for actually finding the “certifying” point $c$. We are unaware of an algorithm for finding Voronoi neighbors that does not involve, in one way or another, constructing the
Voronoi diagram itself. Although there are a number of algorithms for constructing these diagrams—some are presented in §4 of Devadoss and O’Rourke [3]—they are unlikely to be practical for our purposes, except perhaps when $X$ is a Euclidean plane.

A reasonable alternative is to use metric closeness as a kind of approximation for adjacency in the Voronoi sense. Fix some integer $K \geq 2$; given $S \subseteq X$, let $V_x$ denote the family of $K$-sets $V \subseteq S$ that minimize distance to $x$. With reference to (3), then, let

$$V_S(x) = \begin{cases} \emptyset, & \text{if } x \in S \\ \arg\min_{V \in V_x} \text{modefreq}_f(V), & \text{otherwise} \end{cases}.$$  

We say that $V_S(x)$ is the set of $K$-nearest neighbors of $x$ with respect to $S$.

**Lemma 6.** Let $S \subseteq X$ be countable; for any $x \in X - S$, write $S = \{s_1, s_2, \ldots\}$ such that 

$$d(x, s_1) \leq d(x, s_2) \leq \cdots.$$  

If there exists $K \geq 1$ such that $d(x, s_K) < d(x, s_{K+1})$, then for any 

$$0 < \epsilon \leq \frac{1}{2}[d(x, s_{K+1}) - d(x, s_K)]$$

it holds that for all $x' \in B_\epsilon(x)$, $\{s_1, s_2, \ldots, s_K\}$ are the $K$-nearest neighbors of $x'$ with respect to $S$.

**Proof.** For any $x' \in B_\epsilon(x)$ and $1 \leq i \leq K < j$, we have the following:

$$d(x', s_i) \leq d(x', x) + d(x, s_i)$$

$$\leq \epsilon + d(x, s_i) \leq \epsilon + d(x, s_K)$$

$$\leq \frac{1}{2}[d(x, s_{K+1}) - d(x, s_K)] + d(x, s_K)$$

$$= \frac{1}{2}[d(x, s_{K+1}) + d(x, s_K)] = d(x, s_{K+1}) - \frac{1}{2}[d(x, s_{K+1}) - d(x, s_K)]$$

$$\leq d(x, s_{K+1}) - \epsilon \leq d(x, s_j) - \epsilon$$

$$< d(x', s_j).$$

The lemma follows immediately. \hfill \square

**Theorem 7.** Let $\{z_n\}_{n=1}^\infty$ be determined by the process $S(\kappa, \Phi)$ where $\kappa$ is such that, for any $0 < \rho \leq 1$,

$$\sum_{n=1}^\infty \rho^{\kappa(n)} = \infty$$

and $\Phi$ is defined by (3), with $V_S(x)$ denoting $K$-nearest neighbors of $x$ with respect to $S$ ($K \geq 2$). If $x \in X$ is contained in an $f$-contiguous component of positive measure, then $\zeta_n(x) \to f(x)$ with probability one.

---

Note that defining $V_S(x)$ in this way causes $\Phi(x, S) = 0$ when $x \in S$, and otherwise returns the neighbor set that maximizes $\Phi(x, S)$.
Proof. We proceed exactly as in the proof of Theorem 4 up to the identification of the point \( b \) at which the boundary of \( W \) crosses \( C \). For any \( Z_n \), let \( b(n)(i) \in Z_n \) denote the \( i \)-th nearest neighbor of \( b \); that is,

\[
d(b, b(n)(1)) \leq d(b, b(n)(2)) \leq \cdots \leq d(b, b(n)(n)).
\]

Now consider

\[
\epsilon_n = \frac{1}{2} \max_{2 \leq i \leq K} d(b, b(n)(i + 1)) - d(b, b(n)(i)).
\]

Per Lemma 6, any point in \( B_{\epsilon_n}(b) \) will have at least \( b(n)(1) \) and \( b(n)(2) \) among its \( K \)-nearest neighbors with respect to \( Z_n \) (assuming \( \epsilon_n > 0 \)).

Suppose \( \epsilon = \lim inf \epsilon_n > 0 \). As \( b \) is on the boundary of points predicted wrongly infinitely often, there exist \( q_1, q_2 \in B_{\epsilon}(b) \cap X \) such that \( \zeta_n(q_1) \neq \zeta_n(q_2) \) for infinitely many \( n \) (ie, take \( q_1 \) on the \( W \) side and \( q_2 \) on the \( X - W \) side of \( \partial W \)). For these \( n \), it must be that \( f(b(n)(i)) \neq f(b(n)(j)) \) for some \( 1 \leq i < j \leq K \), which implies that \( B_{\epsilon}(b) \cap X \subseteq Q \). We can proceed from here exactly as in the proof of Theorem 4: find \( c \in C \cap B_{\epsilon}(b) \) such that \( c \in W \), etc. (However, see Remark 6.)

If on the other hand \( \epsilon = 0 \), we must fall back upon “brute force” to demonstrate that a sample will eventually be placed arbitrarily close to any point in \( \text{supp}(\mu) \) with probability one. (If one considers the definition of \( \epsilon_n \), however, the case that \( \epsilon = 0 \) seems to defy common sense; Remark 7 clarifies this intuition.)

In any event, the theorem is proved.

\[ \square \]

Corollary. Suppose \( S(\kappa, \Phi) \) is as described by Theorem 7. If \( X \) is separable; the \( f \)-boundary has measure zero; and the union of all \( f \)-contiguous components with measure zero itself has measure zero; then \( \zeta_n \to f \) in measure with probability one.

Remark 5. What is a reasonable value for \( K \)? If we view the \( K \)-nearest neighbors as a kind of approximation of the Voronoi neighbors, then setting \( K \) to the expected number of Voronoi neighbors is reasonable. Suppose \( X \) is an \( m \)-dimensional Euclidean space: letting \( K \) be this expectation, Tanemura [9, 10] reports the exact results

\[
m = 2 \implies K = 6 \\
m = 3 \implies K = \frac{48\pi^2}{35} + 2 = 15.535457 \ldots \\
m = 4 \implies K = \frac{340}{9} = 37.777 \ldots
\]

and derives the value \( K = 88.56 \ldots \) empirically for \( m = 5 \). We are not aware of results for \( m \geq 6 \), although it is reasonable to assume from the preceding that \( K \) grows exponentially in \( m \).

Remark 6. For the same reasons as noted in Remark 4, it is useful that \( \mu(Q) \) be small. Suppose \( X \) is separable, and let \( x \in \text{supp}(\mu) \) be off the \( f \)-boundary. If \( x \in Q \), then there (almost surely) must exist \( \gamma > 0 \) such that \( z_n \notin B_{\gamma}(x) \) for any \( n \). But the Second Borel-Cantelli Lemma tells us that for infinitely many \( n \), all of the \( \kappa(n) \) candidates for \( z_n \) appear in
$B_r(x)$, given that $\mu(B_r(x)) > 0$; so $z_n \in B_r(x)$, which is a contradiction. Thus $x \notin Q$, from which it follows by Lemma\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.} that $\mu(Q) = 0$, provided that the $f$-boundary has measure zero. This is the analogue to Proposition\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.} for the $K$-nearest neighbors variant of the non-modal count heuristic.

Remark 7. Let $b$, $b_n(i)$, $\epsilon_n$, and $\epsilon$ be as in the proof of Theorem\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.}. We have seen that we are forced into a “brute force” method when $\epsilon = 0$; how can this be mitigated? Let $r = \lim_{n \to \infty} d(b, b_n(1))$; since $b$ is not an $f$-boundary point, $r > 0$. Now consider the shells

$$R_n(b) = \{x \in X; r \leq d(b, x) \leq d(b, b_n(K))\}.$$ 

If $\epsilon = 0$, it follows that

$$R(b) = \lim_{n \to \infty} R_n(b) = \{x \in X; d(b, x) = r\}$$

and furthermore $\mu(R_n(b)) \to \mu(R(b))$. Therefore if $\mu(R(b)) = 0$, then $\epsilon > 0$ asymptotically almost always (since otherwise $K$ samples must be placed in a set of ever-decreasing measure). This condition is satisfied if every sphere—that is, every set of points at some fixed distance from a chosen point—has measure zero. This is a very natural hypothesis; e.g., one intuitively expects that every $(n - 1)$-dimensional manifold in an $n$-dimensional space has measure zero.

### 3.3 The $m$ nearest neighbors rule

For clarity of exposition we have used the nearest neighbor rule for prediction, but it is not especially difficult to extend the results to the $m$ nearest neighbors rule for any fixed integer $m > 1$. Given any $S \subseteq X$, let $U_x$ denote the family of $m$-sets $U \subseteq S$ that minimize distance to $x$. Let

$$U_S(x) = \begin{cases} \{x\}, & \text{if } x \in S \\ \arg \min_{U \in U_x} \text{modefreq}_f(U), & \text{otherwise} \end{cases}.$$

Now instead of (1), we use

$$\zeta_n(x) = \text{mode}_f(U_{Z_n}(x))$$

for any $x \in X$, with ties broken uniformly at random.\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.}

Consider the proof of Theorem\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.} given $x \in \text{supp}(\mu)$ off the $f$-boundary, there exists $r > 0$ such that $\mu(B_r(x) - X_{f(x)}) = 0$, and the proof shows that some sample will be appear in $B_r(x)$ almost surely. But in fact the proof, which uses the Second Borel-Cantelli Lemma, establishes that this almost certainly happens infinitely often. In other words, given any $m > 1$, for sufficiently large $n$, almost surely $|B_r(x) \cap Z_n| \geq m$, which implies that $\zeta_n(x) = f(x)$ almost surely. Hence Theorem\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.} is valid under the $m$ nearest neighbors rule.

We can also generalize Theorem\footnote{Note that this definition predicts based on the most ambiguous set of neighbors.} although we must have $K > \lceil m/2 \rceil$. Referring back to the proof, let

$$\epsilon_n = \frac{1}{2} \max_{|m/2| < i \leq K} d(b, b_n(i + 1)) - d(b, b_n(i)).$$
Suppose $\epsilon = \liminf \epsilon_n > 0$. Now any point in $B_\epsilon(b)$ will have $b_n(1), \ldots, b_n([m/2] + 1)$ among its $K$-nearest neighbors per Lemma 6. As in the original proof, we take two points in $B_\epsilon(b) \cap X$ on either side of $\partial W$ and observe that this forces at least one of the $K$-nearest neighbors to have a non-modal $f$-value for infinitely many $n$. This establishes that $B_\epsilon(b) \cap X \subseteq Q$. The rest of the proof proceeds as written, except that we now use the power of the Second Borel-Cantelli Lemma to show that our chosen events occur infinitely often, and can therefore meet any $m$.

Theorem 4 does not seem to be easily generalized, given that the $m$ nearest neighbors have no simply-characterized intersection with the Voronoi neighbors for $m > 1$.

4 Conclusion

In this work we have articulated a general procedure for selective sampling for nearest neighbor pattern classification. This procedure is guided by a selection heuristic $\Phi$, and we proved that the nearest neighbor rule prediction converges pointwise to the true function on the support of the domain under each of the following choices for $\Phi$: distance to sample set ($\S$ 3.1); non-modal count per Voronoi neighbors ($\S$ 3.2.1); and non-modal count per $K$-nearest neighbors ($\S$ 3.2.2). We also established convergence in measure as a corollary, provided that the domain is separable. Finally, we showed that the first and third alternatives for $\Phi$ are also valid under the $m$ nearest neighbors rule for any $m > 1$ ($\S$ 3.3).

There are many avenues for future research; we describe three open problems that seem particularly interesting and valuable.

1. For reasons explained in $\S$ 1, our investigations have taken place in a deterministic setting, as opposed to the more general probabilistic approach taken in the classical results [1, 2]. However, it ought to be possible to recover the probabilistic setting if the concept of an $f$-contiguous component can somehow be generalized to the situation where $f$ is a random variable.

2. Our theorems are silent on the rate of convergence, which is obviously an essential question in practical applications. Intuition and empirical results (such as Figures 1 and 2) suggest that selective sampling converges more quickly than iid sampling, but we cannot say how much more quickly; nor do we yet understand how the prediction error is related to the number of samples.

Kulkarni and Posner [6] derive a number of convergence results for arbitrary sampling in a very general setting. Although these results have limited direct practical impact, since arbitrary sampling may not converge to the true function at all ($\S$ 2.1), they do include bounds on the expected value of the distance of the latest sample from all previous samples, where samples are chosen by a stationary process. Intuitively, this value decreases as the predictions become more accurate. By comparing the rate of decrease under selective sampling versus iid sampling, it may be possible to adduce convergence rates, at least in a relative fashion.
3. What are valid choices for the heuristic $\Phi$? We have given three, but we do not think this is exhaustive. It also occurs to us that the distance to sample set and the two non-modal count heuristics have very different convergence proofs—are there perhaps different classes of selection heuristics that can be identified?

Although these and other questions remain open, we nonetheless believe that the results presented in this paper provide a firm theoretical foundation for the use of selective sampling techniques in practical applications.

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