Diameter-based Interactive Structure Search

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Abstract
In this work, we introduce interactive structure search, a generic framework that encompasses many interactive learning settings, both explored and unexplored. We show that a recently developed active learning algorithm of Tosh & Dasgupta (2017) can be adapted for interactive structure search, that it can be made noise-tolerant, and that it enjoys favorable convergence rates.

1. Introduction
The standard approaches to learning structures from data generally do not incorporate human interaction into the learning process. Typically, a data set is collected and labeled, if appropriate, and an algorithm is run to find the structure that best fits the data. Interactive structure learning, by contrast, adaptively solicits feedback from a human (or other information source) during the structure learning process. The hope is that by incorporating interaction into the learning process, we can learn higher quality structures with potentially less data or lower computational costs.

Recently, there has been interest in designing algorithms for interactive structure learning. Some works have attacked this problem in broad generality, designing algorithms that are capable of interactively learning a broad class of structures (Tosh & Dasgupta, 2018; Emamjomeh-Zadeh & Kempe, 2017). Others have designed structure-specific interactive learning algorithms in a variety of settings, including flat and hierarchical clustering (Wagstaff & Cardie, 2000; Awasthi et al., 2014; Ashtiani et al., 2016; Vikram & Dasgupta, 2016), topic modeling (Hu et al., 2014; Lund et al., 2017), and matrix completion (Krishnamurthy & Singh, 2014). In all of these works, the ultimate goal is to find the structure that a user has in mind, and the algorithms are designed around this objective.

However, it is not always the case that users of interactive learning algorithms are primarily interested in obtaining high-quality estimates of a particular structure. Consider the setting of drug discovery, where there are $n$ cell lines and $p$ drugs under consideration, along with some low-rank matrix $A \in \mathbb{R}^{n \times p}$, where the entry $A_{ij}$ corresponds to the survival rate of the $i$th cell line when exposed to drug $i$. Initially, all the entries of $A$ are unknown, and an experiment must be run to observe an entry. The goal in the drug discovery setting is to find the column $A_j$ that best meets some criteria, measured by a score function $s : \mathbb{R}^p \to \mathbb{R}$, while running as few experiments as possible. In this setting, although the drug that we select may depend on our estimate of $A$, our primary interest is not in obtaining a high-quality estimate of $A$, rather we only care about finding a good drug.

In this work, we introduce interactive structure search, a general framework that encompasses both traditional interactive structure learning as well as other scenarios that, like the drug discovery setting, have objectives that deviate from the estimation problem. We also demonstrate that there is a natural, general-purpose interactive search algorithm, and we give guarantees on its consistency and convergence rates, even in the presence of noise.

2. Interactive structure search
In this section we define the interactive structure search task.

2.1. Structure decompositions
Denote by $\mathcal{G}$ the space of structures under consideration, these could be, for example, binary classifiers, or clusterings of some fixed data set, or low rank $n \times p$ matrices. As in previous work of Tosh & Dasgupta (2018), we will view each structure in $\mathcal{G}$ as a function from a set of fixed atomic questions $\mathcal{A}$ to a set of potential responses $\mathcal{Y}$. Consider the following examples.

- **Binary classifiers.** When $\mathcal{G}$ is a collection of classifiers, each atom $a \in \mathcal{A}$ corresponds to a data point and $\mathcal{Y} = \{0, 1\}$ is the set of labels.
- **Clusterings.** If $\mathcal{G}$ is a set of clusterings of a collection of $n$ items, then we may view $g \in \mathcal{G}$ as the function...
from \( A = \binom{[n]}{2} \) to \( \gamma = \{0, 1\} \), where \( g((i,j)) = 1 \) if \( i, j \) belong to the same cluster in \( g \) and 0 otherwise.

- **Binary hierarchical clusterings.** If \( G \) is a set of binary hierarchies over \( n \) items, then we may view \( g \in G \) as the function from \( A = \binom{[n]}{3} \) to \( \gamma = \{0, 1, 2\} \), where

\[
g((i,j,k)) = \begin{cases} 0 & \text{if } i, j \text{ are clustered before } k \text{ in } g \\
1 & \text{if } i, k \text{ are clustered before } j \text{ in } g \\
2 & \text{otherwise}
\end{cases}
\]

- **Matrices.** If \( G \) is a set of \( n \times p \) matrices, then \( A = [n] \times [p] \) and \( \gamma = \mathbb{R} \), and \( g((i,j)) \) is the \((i,j)\)-th entry of the matrix corresponding to \( g \).

- **Metrics.** If \( G \) is a set of metrics over \( n \) items, then \( A = [n] \times [n] \) and \( \gamma = \mathbb{R}_{\geq 0} \), and \( g((i,j)) \) is the distance between items \( i \) and \( j \) in metric \( G \).

We will also assume that there is some distribution \( D \) over \( A \). In the case of classifiers, \( D \) is the data distribution. For clusterings over a fixed collection of items or matrices of a fixed size, a reasonable choice for \( D \) would be the uniform distribution over \( A \).

### 2.2. Structure distances

We are interested in settings where the goal is not to recover a particular structure but rather to recover some aspect of that structure. We capture this objective in the form of a **structure distance** \( d : G \times G \to \mathbb{R}_{\geq 0} \). If \( g^* \in G \) is some ground-truth structure, then our objective is to find a structure \( g \in G \) such that \( d(g^*, g) \) is small. To see the flexibility of this approach, consider the following examples.

- **Low-error classifiers.** If our objective is to find a classifier with low error, then we may take our distance to be

\[
d(g, g') = \Pr_{x \sim D}(g(x) \neq g'(x)).
\]

This is the standard classification distance used in active learning. More generally, this is the distance used for interactive structure learning in (Tosh & Dasgupta, 2018).

- **Cluster identification.** In some clustering situations, there is some particular node of interest \( i^* \), and our goal is to find the cluster to which \( i^* \) belongs. In this case, we can take our distance function as

\[
d(g, g') = \frac{|C(g, i^*) \Delta C(g', i^*)|}{|C(g, i^*) \cup C(g', i^*)|}
\]

where \( \Delta \) denotes symmetric difference between sets and \( C(g, i) = \{ j \in [n] : g((i, j)) = 1 \} \).

- **Column selection.** If our goal is to find the best column of an \( n \times p \) matrix as measured by some score function \( s : \mathbb{R}^n \to \mathbb{R} \), then we might define our distance as

\[
d(g, g') = \max \{ s(g(\cdot, j_g)) - s(g(\cdot, j_{g'})) ;
\]

\[
s(g'(\cdot, j_{g'})) - s(g'(\cdot, j_g)) \}
\]

where \( g(\cdot, j) \) denotes the \( j \)-th column of \( g \) and \( j_g = \arg \max_j s(g(\cdot, j)) \).

- **Exact structure identification.** If \( G \) is finite and our goal is to exactly identify a structure \( g^* \), then we might take

\[
d(g, g') = \mathbb{I}[g \neq g']
\]

where \( \mathbb{I}[\cdot] \) is the indicator function.

Thus, the structure distance is a flexible way to encode objectives into the structure search problem. Through the remainder of the paper, we assume that we have such a distance \( d(\cdot, \cdot) \), that our objective is to find a \( g \in G \) satisfying \( d(g, g^*) < \epsilon \) for some \( \epsilon > 0 \), and that we can efficiently compute \( d(g, g') \) for any two structures \( g, g' \in G \). We will also assume that \( d(g, g') \leq 1 \), which can be achieved with an appropriate normalization.

### 2.3. The average splitting index

Given a set of structures \( G \) and a suitable distance function, how should we go about finding a structure with low distance to the ground truth? One approach, which Tosh & Dasgupta (2017) proposed for the realizable binary classification setting, is to try to find a distribution over \( G \) such that the structures are close to \( g^* \) on average. We take up their approach again here in our more general and potentially noisy setting.

Let \( \pi \) be some probability measure over \( G \). Define the average diameter of \( \pi \) as

\[
\text{avg-diam}(\pi) = \mathbb{E}_{g, g' \sim \pi}[d(g, g')].
\]

The following result shows that if one can find a distribution \( \pi \) with low average diameter that puts sufficient mass on a target structure \( g^* \), then one can readily find a structure with small distance to \( g^* \) by random sampling.

#### Lemma 1 (Lemma 1 of Tosh & Dasgupta (2017)).

Pick \( g^* \in G \) and let \( \pi \) be a distribution over \( G \), then

\[
\mathbb{E}_{g \sim \pi}[d(g, g^*)] \leq \frac{\text{avg-diam}(\pi)}{\pi(g^*)}.
\]

Lemma 1 reduces the problem of finding a structure close to \( g^* \) to that of finding a low average diameter distribution \( \pi \), provided we can sample from it. Thus, we are interested
in atomic questions whose answers help us find distributions with low average diameter. This motivates the concept of average splitting. For a given subset \( V \subset \mathcal{G} \), let \( \pi|_V \) denote the restriction of \( \pi \) to \( V \), that is
\[
\pi|_V(g) = \frac{\pi(g) \mathbb{1}[g \in V]}{\pi(V)}.
\]

For a given atomic question \( a \in \mathcal{A} \) and possible response \( y \in \mathcal{Y} \), let \( \mathcal{G}_a^y = \{g \in \mathcal{G} : g(a) = y\} \). For any \( a \in \mathcal{A} \), we say that a \( \rho \)-average splits \( \pi \) if
\[
\max_y \pi(\mathcal{G}_a^y)^{avg-diam(\pi|_{\mathcal{G}_a^y})} \leq (1-\rho)avg-diam(\pi). \quad (1)
\]

Additionally, we say that \( \pi \) is \((\rho, \tau)\)-average splittable if
\[
\Pr_{a \sim \mathcal{D}}(a \rho\text{-average splits } \pi) \geq \tau.
\]

Finally, we say that \( \mathcal{G} \) has average splitting index \((\rho, \epsilon, \tau)\) if any distribution \( \pi \) over \( \mathcal{G} \) satisfying \( \text{avg-diam}(\pi) > \epsilon \) is \((\rho, \tau)\)-average splittable.

Given an efficient sampler for \( \pi \), we can estimate all of the relevant quantities in equation (1) via Monte Carlo approximations. For a sequence of structure pairs \( E = \{(g_1, g_1'), \ldots, (g_n, g_n')\} \in \mathbb{G}^{2 \times n} \), define
\[
\psi(E) = \sum_{i=1}^n d(g_i, g_i').
\]

When the structure pairs \( g_i, g_i' \) are drawn i.i.d. from \( \pi \), the following identities hold for any \( a \in \mathcal{A} \) and \( y \in \mathcal{Y} \):
\[
\frac{1}{n} \mathbb{E}[\psi(E)] = \text{avg-diam}(\pi)
\]
\[
\frac{1}{n} \mathbb{E}[\psi(E^g_a)] = \pi(\mathcal{G}_a^y)^{2\text{avg-diam}(\pi|_{\mathcal{G}_a^y})}
\]

Where we define \( E^g_a = \{(g, g') \in E : g(a) = y = g'(a)\} \).

In the case where \( \mathcal{G} \) is a binary hypothesis class with average splitting index \((\rho, \epsilon, \tau)\), Tosh & Dasgupta (2017) gave a simple algorithm that can efficiently find a query to \( O(\rho) \)-average split any distribution \( \pi \) with average diameter \( \epsilon \) while sampling \( O(1/\epsilon^2 + 1/\text{avg-diam}(\pi)^2) \) structures from \( \pi \). In Algorithm 2, we present an algorithm based on inverse sampling (Haldane, 1945) that enjoys the same guarantees in our more general setting while sampling fewer structures.

**Lemma 2.** Pick \( \alpha > 0 \). If \textsc{select} is run with atoms \( a_1, \ldots, a_m \), one of which \( \rho \)-average splits \( \pi \), then with probability \( 1 - \delta \), \textsc{select} returns a data point that \((1 - \alpha)\rho\)-average splits \( \pi \) while drawing no more than
\[
\frac{12}{\alpha^2(1-\alpha)\rho \text{avg-diam}(\pi)} \log \frac{m + |\mathcal{Y}|}{\delta}
\]
pairs of hypotheses in total.

The proof of Lemma 2 is deferred to the appendix.

### 3. Diameter-based structure search

The approach of Tosh & Dasgupta (2017) in the noiseless and realizable binary classification setting was to maintain a distribution \( \pi_t \) over all structures that are consistent with the feedback observed so far. In our setting, this corresponds to updating the distribution as
\[
\pi_t(g) \propto \pi_{t-1}(g) \mathbb{1}[g(a_t) = y_t]
\]
after querying \( a_t \) and receiving label \( y_t \).

In this work, we want to be able to handle settings where our measurements or responses are noisy or inconsistent with a ground-truth structure. Thus, we consider a ‘softer’ posterior update:
\[
\pi_t(g) \propto \pi_{t-1}(g) \exp(-\beta \mathbb{1}[g(a_t) \neq y_t])
\]
where \( \beta > 0 \) is some parameter corresponding roughly to our confidence in the accuracy of the responses. Note that by taking \( \beta \to \infty \), we recover the update in equation (2).

The update in equation (3) has been shown to enjoy favorable guarantees for active learning strategies that attempt to shrink \( \pi \)-mass (Nowak, 2011; Tosh & Dasgupta, 2018). We will show that it also works well for our algorithm, NDBAL, which attempts to shrink the average diameter. The full algorithm for NDBAL is displayed in Algorithm 1.

#### 3.1. Consistency

In what follows, we will make the simplifying assumption that \( \mathcal{A} \) is some large, but finite space. Since structures in \( \mathcal{G} \) are identifiable by their responses to elements of \( \mathcal{A} \), this implies that \( \mathcal{G} \) is also finite. This assumption will be relaxed later when we study fast rates of convergence.

Our goal in this section is to demonstrate consistency of NDBAL. In our context, we will take this to mean
\[
\lim_{t \to \infty} \mathbb{E}_{g \sim \pi}[d(g, g^*)] = 0
\]
almost surely, where \( g^* \in \mathcal{G} \) is some ground truth structure. Notice that at each time \( t \), the random outcomes consist of the atom \( a_t \) presented to the user as well as the response \( y_t \) to \( a_t \). Let \( \mathcal{F}_t \) denote the sigma-field of all outcomes up to and including time \( t \).

In order to demonstrate consistency, we will need to make a few assumptions on our problem setup. Our first assumption will be that any two structures with positive distance ought to be distinguished with positive probability by a random atom.

**Assumption 1.** For any \( g, g' \in \mathcal{G} \) such that \( d(g, g') > 0 \), we have \( \Pr_{a \sim \mathcal{D}}(g(a) \neq g'(a)) > 0 \).

We will also need to make an assumption on the typical responses provided by a user. Let \( \eta(y \mid a) \) denote the conditional probability that a user provides response \( y \) to atomic
Algorithm 1 NDBAL

Input: Prior distribution over \( G \), \( \beta > 0 \)
Initialize \( \pi_0 = \pi \)
for \( t = 1, 2, \ldots \) do
  Draw \( m \) atomic questions \( a = (a_1, \ldots, a_m) \)
  Query \( a = \text{SELECT}(\pi, a) \) and receive label \( y \)
  \( \pi_t(g) \propto \pi_{t-1}(g) \exp(-\beta \mathbb{1}[g(a) \neq y]) \)
end for
return Posterior \( \pi_t \)

Algorithm 2 SELECT

Input: Distribution \( \pi \), atoms \( a_1, \ldots, a_m \), and \( \epsilon, \delta \in (0, 1) \)
Set \( N = \frac{\ln(2\epsilon\epsilon)}{m^2|G|}, T = 0, S^{a_i y}_T = 0 \)
for \( T = 1, 2, \ldots \) do
  Draw \( g, g' \sim \pi \) and compute for all \( a_i, y: \)
  \( S^{a_i y}_T = S^{a_i y}_{T-1} + d(h, h')(1 - \mathbb{1}[g(a_i) = y = g'(a_i)]) \)
  If \( \exists a_i, s.t. S^{a_i y}_T \geq N \) for all \( y \in \mathcal{Y}, \text{halt} \) and return \( a_i \).
end for

Question \( a \). We will require that when we query an atomic question, the most likely response we observe is the true label.

Assumption 2. There exists \( g^* \in G \) and \( \lambda > 0 \) such that \( \eta(g^*(a)) \mid a \geq \eta(y) \mid a + \lambda \) for any \( a \in A \) and \( y \neq g^*(a) \).

In the setting where \( G \) is a collection of binary classifiers, Assumption 2 is equivalent to Massart’s bounded noise condition (Awasthi et al., 2015).

Our analysis will focus on the behavior of the potential function \( \text{avg-diam(} \pi_t \)/\( \pi_t(g^*) \) \). Note that by Lemma 1, this potential function has the lower bound

\[
E_{g \sim \pi_t}[d(g, g^*)] \leq \frac{\text{avg-diam(} \pi_t \)}{\pi_t(g^*)}.
\]

Thus, demonstrating that this potential function goes to 0 almost surely implies consistency. The following lemma, whose proof is deferred to the appendix, demonstrates that under Assumption 2, a related potential function is guaranteed to decrease in expectation.

Lemma 3. Pick \( k \geq 2 \). Suppose Assumption 2 holds and \( \beta \leq \lambda/(2 + 2k^2) \). If we query an atom \( a_t \) that \( \rho \)-average splits \( \pi_{t-1} \), then in expectation over the randomness of the user’s response, we have

\[
E\left[ \frac{\text{avg-diam(} \pi_t \)}{\pi_t(g^*)^k} \mid F_{t-1}, a_t \right] = (1 - \Delta) \frac{\text{avg-diam(} \pi_{t-1} \)}{\pi_{t-1}(g^*)^k}
\]

where \( \Delta \geq \rho \lambda \beta / 2 \).

Lemma 3 tells us that at each round, our potential function decreases in expectation, for an appropriate choice of \( \beta \). However, this does not tell us how \( \text{avg-diam(} \pi_t \) and \( \pi_t(g^*) \) behave individually. The following lemma, whose proof appears in the appendix, shows that \( 1/\pi_t(g^*) \) is well-behaved.

Lemma 4. Pick \( k \geq 1 \). Suppose Assumption 2 holds and \( \beta \leq \lambda/k \). Then for any query \( a_t \), we have

\[
E\left[ \frac{1}{\pi_t(g^*)^k} \mid F_{t-1}, a_t \right] \leq \frac{1}{\pi_{t-1}(g^*)^k}.
\]

The following lemma, whose proof appears in the appendix, demonstrates that we can lower bound the expected splitting of the data points chosen by DBAL.

Lemma 5. If Assumption 1 holds, then there is a constant \( c > 0 \) such that for every round \( t \), DBAL chooses a point that \( \rho_t \)-average split \( \pi_t \) satisfying \( E[\rho_t \mid F_{t-1}] \geq c \log \frac{\pi_{t-1}(g^*)}{\pi_{t-1}(g^*)} \).

We are now ready to prove consistency of DBAL.

Theorem 6. If Assumption 2 holds, \( \beta \leq \lambda/10 \), and \( \pi_1(g^*) > 0 \), then \( E_{g \sim \pi_1}[d(g, g^*)] \rightarrow 0 \) almost surely.

Proof. Let \( X_t = \text{avg-diam}(\pi_t) \) and \( Y_t = 1/\pi_t(g^*)^2 \). Since \( \beta \leq \lambda/10 \), Lemmas 3 and 5, together with the inequality \( x/\log(1/x) \geq x^2 \) for \( x \in (0, 1) \), imply

\[
E[X_t Y_t \mid F_{t-1}] \leq X_{t-1} Y_{t-1} - c X_{t-1}^2 Y_{t-1}
\]

for some constant \( c > 0 \). Since \( X_t Y_t \) and \( Y_t \) are positive supermartingales, we have that \( X_t Y_t \rightarrow Z \) and \( Y_t \rightarrow Y \) for some random variables \( Z, Y \) almost surely. Moreover, since \( Y_t \rightarrow Y \) almost surely, we have \( X_t^2 Y_t \rightarrow W \) for some random variable \( W \) almost surely.

Iterating expectations in equation (4) and using the fact that \( X_t Y_t \geq 0 \), we have

\[
0 \leq E[X_t Y_t] \leq \frac{\text{avg-diam(} \pi_1 \)}{\pi_1(g^*)^2} - c \sum_{i=1}^{t-1} E[X_i^2 Y_i].
\]

In particular, we know \( \lim_{t \rightarrow \infty} E[X_t^2 Y_t] = 0 \). By Fatou’s lemma, this implies

\[
0 \leq E \left[ \lim_{t \rightarrow \infty} X_t^2 Y_t \right] \leq \lim_{t \rightarrow \infty} E[X_t^2 Y_t] = 0.
\]

Thus, we have

\[
\lim_{t \rightarrow \infty} \frac{\text{avg-diam(} \pi_t \)}{\pi_t(g^*)^2} = \lim_{t \rightarrow \infty} X_t^2 Y_t = 0
\]

almost surely. By the Continuous Mapping Theorem, this implies \( \frac{\text{avg-diam(} \pi_t \)}{\pi_t(g^*)} \rightarrow 0 \) almost surely. Since

\[
0 \leq E_{g \sim \pi_t}[d(g, g^*)] \leq \frac{\text{avg-diam(} \pi_t \)}{\pi_t(g^*)},
\]
we have the theorem statement.

### 3.2. Convergence rates

We now turn to a setting where there is some fixed error threshold $\epsilon > 0$, and our goal is to find a distribution $\pi_t$ satisfying $\mathbb{E}_{g \sim \pi_t} [d(g, g^*)] < \epsilon$. The following theorem provides a bound on the resources that NDBAL requires to find such a distribution.

**Theorem 7.** Let $\epsilon, \delta > 0$ and $\epsilon_o = \epsilon \sigma(\pi^*)/4$. Suppose that the user’s feedback satisfies Assumption 2 and $\mathcal{G}$ has average splitting index $(\rho, \epsilon, \tau)$. If NDBAL is run with $\beta \leq \lambda/10$, then with probability $1 - \delta$, DBAL encounters a posterior distribution $\pi_t$ satisfying avg-diam($\pi_t$)/$\pi_t(g^*)^2 \leq \epsilon$ before using the following resources:

- $T \leq \frac{8}{\rho \lambda (1 - \beta)} \max \left( \ln \frac{1}{\epsilon \pi(\pi^*)^2}, \frac{8 \delta^2}{\rho \lambda (1 - \beta)} \ln \frac{1}{\delta} \right)$ rounds, with one label requested per round,
- $m \leq \frac{1}{\epsilon} \log \frac{2T}{\delta}$ unlabeled data points drawn per round, and
- $n \leq O \left( \frac{1}{\epsilon \sigma} \log \frac{(m+\left|\mathcal{G}\right|)T}{\delta} \right)$ structures sampled per round.

**Proof.** From Lemma 4, we know that $1/\pi_t(g^*)$ is a positive supermartingale when $\beta \leq \lambda/2$. From standard martingale theory (Rensnick, 2013), we have $\pi_t(g^*)^2 \geq \delta \pi(g^*)^2/4$ with probability at least $1 - \delta/4$.

Conditioned on this event, we have by a union bound that if we sample $m = \frac{1}{\epsilon} \log \frac{2T}{\delta}$ data points at every round, then with probability $1 - \delta/4$, one of those data points will $\rho$-average split $\pi_t$ for every round in which avg-diam($\pi_t$)/$\pi_t(g^*)^2 > \epsilon$. Conditioned on drawing such points, Lemma 2 tells us that SELECT terminates with a data point that $\rho/8$-average splits $\pi_t$ with probability $1 - \delta/4$ after drawing $n$ hypotheses, for the value of $n$ given in the statement.

Let us condition on all of these events happening. For round $t$ define the random variable

$$\Delta_t = 1 - \frac{\text{avg-diam}(\pi_t)}{\pi_t(g^*)^2} \cdot \frac{\pi_{t-1}(g^*)^2}{\text{avg-diam}(\pi_{t-1})}.$$  

If $\pi_{t-1}$ satisfies $\text{avg-diam}(\pi_{t-1})/\pi_{t-1}(g^*)^2 > \epsilon$, then the query $x_t$ $\rho/8$-average splits $\pi_{t-1}$. By Lemma 3,  

$$\mathbb{E}[\Delta_t | F_{t-1}] \geq \frac{1}{8} \rho \lambda \beta (1 - \beta).$$

Now suppose by contradiction that $\text{avg-diam}(\pi_t)/\pi_t(g^*)^2 > \epsilon$ for $t = 1, \ldots, T$. Then we have $\mathbb{E}[\Delta_1 + \ldots + \Delta_T] \geq \frac{1}{8} \rho \lambda \beta (1 - \beta)$. To see that this sum is concentrated about its expectation, we notice that $\Delta_t \in \left[ 1 - e^{2\beta}, 1 \right]$ since  

$$e^{-2\beta} \pi_{t-1}(g^*) \leq \pi_t(g^*) \leq e^{2\beta} \pi_{t-1}(g^*)$$

for all $g \in \mathcal{G}$ which implies  

$$e^{-2\beta} \leq \frac{\text{avg-diam}(\pi_t)}{\pi_t(g^*)^2} \cdot \frac{\pi_{t-1}(g^*)^2}{\text{avg-diam}(\pi_{t-1})} \leq e^{2\beta}.$$  

By the Azuma-Hoeffding inequality (Azuma, 1967; Hoeffding, 1963), if $T$ achieves the value in the theorem statement, then with probability $1 - \delta$,  

$$\Delta_1 + \ldots + \Delta_T > \frac{1}{2} \mathbb{E}[\Delta_1 + \ldots + \Delta_T] \geq \frac{T}{8} \rho \lambda \beta (1 - \beta) \geq \frac{1}{\epsilon \pi(g^*)^2}.$$  

However, this is a contradiction since  

$$\epsilon < \frac{\text{avg-diam}(\pi_T)}{\pi_T(g^*)^2} = (1 - \Delta_1) \cdots (1 - \Delta_T) \frac{\text{avg-diam}(\pi)}{\pi(g^*)^2} \leq \exp \left( -\frac{1}{\pi(g^*)^2} \right).$$

Thus, with probability $1 - \delta$, we must have encountered a distribution $\pi_t$ in some round $t = 1, \ldots, T$ satisfying $\text{avg-diam}(\pi_t)/\pi_t(g^*)^2 \leq \epsilon$.

While Theorem 7 does provide rates of convergence, it has several issues.

(i) The number of structures that we need to sample in each round depends polynomially on $1/\pi(g^*)$. Not only can this quantity be very large, but we do not a priori know its value.

(ii) Theorem 7 only guarantees that some posterior we encounter will satisfy $\text{avg-diam}(\pi_t)/\pi_t(g^*)^2 < \epsilon$; in particular, it does not tell us how to detect which posterior satisfies this property.

(iii) The average splitting index $(\rho, \epsilon_o, \tau)$ depends on $\pi(g^*)$. In settings where the average splitting index has been bounded (Dasgupta, 2005; Tosh & Dasgupta, 2017), $\rho$ and $\tau$ depend on $\epsilon_o$, meaning that both the label and unlabeled complexity grow as $\pi(g^*)$ shrinks.

Without any further assumptions, issues (i) and (iii) are unavoidable even in the noiseless setting. To see why, consider a setting in which our prior only puts mass on two structures $g$ and $g^*$ where $d(g, g^*) \approx 1$. With access only to a sampling oracle, detecting that there are two structures with positive probability mass requires $\Omega(1/\pi(g^*))$ samples. Moreover, in this scenario we have  

$$\text{avg-diam}(\pi)/\pi(g^*) > \epsilon/2 \rightarrow \mathbb{E}_{g \sim \pi}[d(g, g^*)] > \epsilon.$$  

Thus, with no further assumptions, we need to incur computational and data complexity costs that depend on $\pi(g^*)$.  


3.3. Faster convergence rates

As discussed above, when $g^*$ is completely independent of our prior $\pi$, NDBAL incurs high computational and data complexity costs. To avoid this, we make an assumption on the distribution of $g^*$.

**Assumption 3.** There exists a $\lambda \geq 1$ and distribution $\nu$ over $G$ such that the true structure $g^*$ is drawn from $\nu$ and $1/\lambda \leq \nu(g)/\pi(g) \leq \lambda$ for every $g \in G$.

Assumption 3 is a slight relaxation of the traditional Bayesian assumption. Here we do not require $g^*$ to be drawn from $\pi$ itself, but rather only that it is drawn from some distribution that is close to $\pi$. This relaxed Bayesian assumption can be found in the label complexity analysis of the query-by-committee algorithm (Freund et al., 1997).

Assumption 3 immediately adds more structure to the problem. In particular, if we receive query/label pairs $(a_1, y_1), \ldots, (a_t, y_t)$ where the noise level at $a_i$ is $q_i$, then there is a true posterior distribution which takes the form

$$\nu_t(g) = \frac{1}{Z_t} \nu(g) \exp \left(-\sum_{i=1}^t I[g(a_i) \neq y_i] \ln \frac{1}{q_i} \right)$$

where $Z_t$ is the normalizing constant to make the above sum to one. Without access to $\nu$ and the noise levels $q_i$, there is no way to compute $\nu_t$ directly. However, we may still hope that a random draw from our distribution $\pi_t$ is close to a random draw from $\nu_t$, i.e. that the quantity

$$D(\pi_t, \nu_t) = \mathbb{E}_{g \sim \pi_t, g' \sim \nu_t} [d(h, h')]$$

is small. Thus, our new objective is to show $\pi_t$ satisfies $D(\pi_t, \nu_t) \leq \epsilon$ after relatively few rounds $t$.

Unfortunately, Assumption 3 alone is not capable of ensuring that we can run NDBAL efficiently. To see why, suppose that $\beta$ is set to some conservatively small value but the true noise rates of the points we query are very small, say exponentially small. Then after a few queries, our distribution $\pi_t$ will remain relatively close to $\pi$, but the true posterior $\nu_t$ will differ wildly from $\nu$. Indeed, it may be concentrated on values that have low probability under $\pi$, which brings up the same issues from above that we had hoped to avoid.

To avoid this issue, we will consider the noiseless setting. In this case, we will run NDBAL with $\beta = \infty$ and get the posterior update in equation (2). Within this noiseless and Bayesian setting, we can relax the requirement that $G$ is finite. Instead, we will require that $G$ has bounded graph dimension.

**Definition 8.** Let $S = \{a_1, \ldots, a_m\}$ be a set of atomic questions. We say $G$ G-shatters $S$ if there exists $f : S \rightarrow Y$ such that for all $T \subset S$, there exists $g_T \in G$ satisfying

$$g_T(x) = \begin{cases} f(x) & \text{for all } x \in T \\ \neq f(x) & \text{for all } x \in S \setminus T \end{cases}$$

The graph dimension of $G$ is the size of the largest $S$ such that $G$ G-shatters $S$.

Given the above, we have the following theorem on the performance of NDBAL.

**Theorem 9.** Suppose $G$ has average splitting index $(\rho, \epsilon/(2\lambda^2), \tau)$ and graph dimension $d_G$. If Assumption 3 holds and the noise rate is zero then with probability $1 - \delta$, NDBAL terminates with a distribution $\pi_t$ satisfying $D(\pi_t, \nu_t) \leq \epsilon$ while using the following resources:

(a) $T \leq O \left( \frac{d_G \log |Y|}{\rho} \right)$ rounds with one label per round.

(b) $n_t \leq \frac{1}{\epsilon^2} \log \frac{\tau^2}{3\delta}$ unlabeled data points drawn per round, and

(c) $n \leq O \left( \frac{1}{\epsilon^2} \log \frac{(m+|Y|^2\tau^2)}{\delta} \right)$ structures sampled per round.

The proof of Theorem 9 is deferred to the appendix.

**References**

Angluin, D. and Valiant, L. Fast probabilistic algorithms for hamiltonian circuits and matchings. In *Proceedings of the ninth annual ACM symposium on Theory of computing*, pp. 30–41. ACM, 1977.

Ashtiani, H., Kushagra, S., and Ben-David, S. Clustering with same-cluster queries. In *Advances in Neural Information Processing Systems*, pp. 3216–3224, 2016.

Awasthi, P., Balcan, M.-F., and Voevodski, K. Local algorithms for interactive clustering. In *Proceedings of the 31st International Conference on Machine Learning*, 2014.

Awasthi, P., Balcan, M.-F., Haghitalab, N., and Urner, R. Efficient learning of linear separators under bounded noise. In *Proceedings of the 28th Annual Conference on Learning Theory*, pp. 167–190, 2015.

Azuma, K. Weighted sums of certain dependent random variables. *Tohoku Mathematical Journal, Second Series*, 19(3):357–367, 1967.

Dasgupta, S. Coarse sample complexity bounds for active learning. In *Advances in Neural Information Processing Systems*, 2005.

Emamjomeh-Zadeh, E. and Kempe, D. A general framework for robust interactive learning. In *Advances in Neural Information Processing Systems*, pp. 7082–7091, 2017.
Diameter-based interactive structure search

Freund, Y., Seung, H., Shamir, E., and Tishby, N. Selective sampling using the query by committee algorithm. *Machine Learning*, 28(2):133–168, 1997.

Haldane, J. On a method of estimating frequencies. *Biometrika*, 33(3):222–225, 1945.

Haussler, D. and Long, P. M. A generalization of Sauer’s lemma. *Journal of Combinatorial Theory, Series A*, 71(2):219–240, 1995.

Hoeffding, W. Probability inequalities for sums of bounded random variables. *Journal of the American statistical association*, 58(301):13–30, 1963.

Hu, Y., Boyd-Graber, J., Satinoff, B., and Smith, A. Interactive topic modeling. *Machine Learning*, 95:423–469, 2014.

Krishnamurthy, A. and Singh, A. On the power of adaptivity in matrix completion and approximation. *arXiv preprint arXiv:1407.3619*, 2014.

Lund, J., Cook, C., Seppi, K., and Boyd-Graber, J. Tandem anchoring: A multiword anchor approach for interactive topic modeling. In *Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics*, volume 1, pp. 896–905, 2017.

Nowak, R. The geometry of generalized binary search. *IEEE Transactions on Information Theory*, 57(12):7893–7906, 2011.

Resnick, S. *A probability path*. Springer Science & Business Media, 2013.

Tosh, C. and Dasgupta, S. Diameter-based active learning. In *Proceedings of the 34th International Conference on Machine Learning*, pp. 3444–3452, 2017.

Tosh, C. and Dasgupta, S. Interactive structure learning with structural query-by-committee. In *Advances in Neural Information Processing Systems*, 2018.

Vikram, S. and Dasgupta, S. Interactive Bayesian hierarchical clustering. In *Proceedings of the 33rd International Conference on Machine Learning*, 2016.

Wagstaff, K. and Cardie, C. Clustering with instance-level constraints. In *Proceedings of the 17th International Conference on Machine Learning*, 2000.
A. Proofs from Section 2

A.1. Proof of Lemma 2

To prove Lemma 2, we will appeal to the following multiplicative Chernoff-Hoeffding bound due to Angluin & Valiant (1977).

**Lemma 10.** Let $X_1, \ldots, X_n$ be i.i.d. random variables taking values in $[0, 1]$ and let $X = \sum X_i$ and $\mu = \mathbb{E}[X]$. Then for $0 < \beta < 1$,

(i) $\Pr(X \leq (1 - \beta)\mu) \leq \exp\left(-\frac{\beta^2\mu}{2}\right)$ and

(ii) $\Pr(X \geq (1 + \beta)\mu) \leq \exp\left(-\frac{\beta^2\mu}{3}\right)$.

The key observation to proving Lemma 2 is that if a $\rho$-average split $\pi$, then for all $y \in \mathcal{Y}$ we have

$$\text{avg-diam}(\pi) - \pi(G^y_n)^2\text{avg-diam}(\pi|G^y_n) \geq \rho \text{avg-diam}(\pi).$$

On the other hand, if $a$ does not $\rho$-average split $\pi$, then there is some $y \in \mathcal{Y}$ such that

$$\text{avg-diam}(\pi) - \pi(G^y_n)^2\text{avg-diam}(\pi|G^y_n) < \rho \text{avg-diam}(\pi).$$

Moreover, if $g, g' \sim \pi$, then

$$\mathbb{E}[d(g, g')(1 - \mathbb{1}[g(a) = y = h'(a)])] = \text{avg-diam}(\pi) - \pi(G^y_n)^2\text{avg-diam}(\pi|G^y_n).$$

Using these facts, along with Lemma 10, we have the following result.

**Lemma 2.** Pick $\alpha > 0$. If `SELECT` is run with atoms $a_1, \ldots, a_m$, one of which $\rho$-average splits $\pi$, then with probability

$$1 - \delta, \text{SELECT returns a data point that } (1 - \alpha)\rho\text{-average splits } \pi \text{ while drawing no more than}$$

$$\frac{12}{\alpha^2(1 - \alpha)\rho \text{avg-diam}(\pi)} \log rac{m + |\mathcal{Y}|}{\delta}$$

pairs of hypotheses in total.

**Proof.** Define $T^a_{N, y} = \inf \{n : S^a_{n, y} \geq N\}$. Recalling that $S^a_{n, y} = \sum_{i=1}^n d(g_i, g'_i)(1 - \mathbb{1}[g_i(a) = y = g'_i(a)])$, we have the following relationship between $T^a_{N, y}$ and $S^a_{n, y}$.

$$\Pr(T^a_{N, y} \leq n) = \Pr(S^a_{n, y} \geq N \text{ for some } n_0 \leq n) \leq \Pr(S^a_{n, y} \geq N)$$

$$\Pr(T^a_{N, y} > n) = \Pr(S^a_{n, y} < N \text{ for all } n_0 \leq n) \leq \Pr(S^a_{n, y} < N)$$

Now let $a^*$ be the atom that $\rho$-average splits $\pi$. Then for all $y \in \mathcal{Y}$, we have

$$\Pr \left( T^{a^*}_{N, y} > \frac{N}{(1 + \epsilon/2)(1 - \epsilon/2)\rho \text{avg-diam}(\pi)} \right) \leq \exp \left( -\frac{N\epsilon^2(1 + \epsilon)^2}{8(1 - \epsilon(1 + \epsilon)/2)} \right).$$

On the other hand we know for any data point $a$ that does not $(1 - \epsilon)\rho$-average split $\pi$, there is some $y \in \mathcal{Y}$ such that

$$\Pr \left( T^{a, y}_{N, y} \leq \frac{N}{(1 + \epsilon/2)(1 - \epsilon/2)\rho \text{avg-diam}(\pi)} \right) \leq \exp \left( -\frac{N\epsilon^2}{12(1 - \epsilon/2)} \right).$$

Taking a union bound over $\mathcal{Y}$ and all the $a$'s, we have

$$\Pr (\text{we choose } a_t \text{ that does not } (1 - \epsilon)\rho\text{-average split } \pi) \leq |\mathcal{Y}| \exp \left( -\frac{N\epsilon^2}{4(2 - \epsilon)} \right) + m \exp \left( -\frac{N\epsilon^2}{6(2 + \epsilon)} \right).$$

By our choice of $N$, this is less than $\delta$. \qed
B. Proofs from Section 3

B.1. Proof of Lemma 3

Lemma 3. Pick $k \geq 2$. Suppose Assumption 2 holds and $\beta \leq \lambda/(2 + 2k^2)$. If we query an atom $a_t$ that $\rho$-average splits $\pi_{t-1}$, then in expectation over the randomness of the user’s response, we have

$$
\mathbb{E} \left[ \frac{\text{avg-diam}(\pi_t)}{\pi_t(g^*)^k} \bigg| F_{t-1}, a_t \right] = (1 - \Delta) \frac{\text{avg-diam}(\pi_{t-1})}{\pi_{t-1}(g^*)^k}
$$

where $\Delta \geq \rho \lambda \beta / 2$.

Proof. To simplify notation, take $\pi = \pi_{t-1}$. Suppose that we query $a \in \mathcal{A}$. Enumerate the potential responses as $\mathcal{Y} = \{y_1, y_2, \ldots, y_m\}$. The definition of average splitting implies that there exists a symmetric matrix $R \in [0, 1]^{m \times m}$ satisfying

- $R_{ii} \leq 1 - \rho$ for all $i$,
- $\sum_{j} R_{ij} = 1$, and
- $R_{ij} \text{avg-diam}(\pi) = \sum_{g \in G_a^{y_i}, g' \in G_a^{y_j}} \pi(g)\pi(g')d(g, g')$.

Let us assume w.l.o.g. that $g^*(a) = y_1$. Define the quantity

$$
Q_a^i := \pi(G_a^{y_i}) + e^{-\beta} \sum_{j \neq i} \pi(G_a^{y_j}) = \pi(G_a^{y_i}) + e^{-\beta} (1 - \pi(G_a^{y_i})) \leq 1.
$$

We now derive the form of $\text{avg-diam}(\pi_t)$. In the event that $y_t = i$, we have

$$
\text{avg-diam}(\pi_t) = \sum_{h, h' \in \mathcal{H}} \pi_t(h)\pi_t(h')d(h, h')
$$

$$
= \left( \frac{1}{Q_a^i} \right)^2 \left( \sum_{g, g' \in G_a^{y_i}} \pi(g)\pi(g')d(g, g') + 2e^{-\beta} \sum_{j \neq i} \sum_{g \in G_a^{y_i}, g' \in G_a^{y_j}} \pi(g)\pi(g')d(g, g') \right)
$$

$$
+ e^{-2\beta} \sum_{j \neq i, k \neq i} \sum_{g \in G_a^{y_i}, g' \in G_a^{y_j}} \pi(g)\pi(g')d(g, g')
$$

$$
= \left( \frac{1}{Q_a^i} \right)^2 \left( R_{ii} + 2e^{-\beta} \sum_{j \neq i} R_{ij} + e^{-2\beta} \sum_{j \neq i, k \neq i} R_{jk} \right) \text{avg-diam}(\pi)
$$

$$
= \left( \frac{1}{Q_a^i} \right)^2 \left( R_{ii} + 2e^{-\beta} \sum_{j \neq i} R_{ij} + e^{-2\beta} \left( 1 - R_{ii} - 2 \sum_{j \neq i} R_{ij} \right) \right) \text{avg-diam}(\pi)
$$

$$
= \left( \frac{1}{Q_a^i} \right)^2 \left( e^{-2\beta} + (1 - e^{-2\beta}) R_{ii} + 2(e^{-\beta} - e^{-2\beta}) \sum_{j \neq i} R_{ij} \right) \text{avg-diam}(\pi)
$$

We can also derive the form of $\frac{1}{\pi_t(g^*)^k}$.

$$
\frac{1}{\pi_t(g^*)^k} = \begin{cases} 
\left( \frac{Q_a^i}{\pi_t(g^*)} \right)^k & \text{if } y_t = y_1 \\
\left( \frac{Q_a^i}{e^{-\beta}\pi_t(g^*)} \right)^k & \text{if } y_t = y_i \neq y_1 
\end{cases}
$$
Denoting $\eta(y_i | a) = \gamma_i$ and assuming w.l.o.g. that $\gamma_1 > \gamma_2 \geq \gamma_3 \geq \cdots$, we have

$$\Delta_t := \frac{\pi(g^*)^k}{\text{avg-diam}(\pi)} \cdot \mathbb{E} \left[ \frac{\text{avg-diam}(\pi_t)}{\pi_t(g^*)^k} \right] = \gamma_1(Q_1^k)^{k-2} \left( e^{-2\beta} + (1 - e^{-2\beta})R_{11} + 2(e^{-\beta} - e^{-2\beta}) \sum_{j \neq 1} R_{1j} \right)$$

$$+ \sum_{i \geq 2} \gamma_i(Q_i^k)^{k-2} e^{k\beta} \left( e^{-2\beta} + (1 - e^{-2\beta})R_{ii} + 2(e^{-\beta} - e^{-2\beta}) \sum_{j \neq i} R_{ij} \right)$$

$$\leq (1 - \gamma_1)e^{(k-2)\beta} + \gamma_1 \left( e^{-2\beta} + (1 - e^{-2\beta})R_{11} + 2(e^{-\beta} - e^{-2\beta}) \sum_{j \neq 1} R_{1j} \right)$$

$$+ \gamma_2 \left( e^{k\beta} - e^{(k-2)\beta} \sum_{i \geq 2} R_{ii} + 2(e^{(k-1)\beta} - e^{(k-2)\beta}) \sum_{i \geq 2} \sum_{j \neq i} R_{ij} \right)$$

$$\leq (1 - \gamma_1)e^{(k-2)\beta} + \gamma_1(1 - e^{-2\beta})R_{11} + \gamma_2(e^{k\beta} - e^{(k-2)\beta}) \sum_{i \geq 2} R_{ii}$$

$$+ \left( \gamma_1(e^{-\beta} - e^{-2\beta}) + \gamma_2(e^{(k-1)\beta} - e^{(k-2)\beta}) \right) \left( 1 - \sum_{i \geq 1} R_{ii} \right)$$

Using the inequalities $1 + x \leq e^x \leq 1 + x + x^2$ for $|x| \leq 1$ and Assumption 2, we can verify that the following inequalities hold for our choice of $\beta$:

$$\gamma_2(e^{k\beta} - e^{(k-2)\beta}) \leq \gamma_1(e^{-\beta} - e^{-2\beta}) + \gamma_2(e^{(k-1)\beta} - e^{(k-2)\beta}) \leq \gamma_1(1 - e^{-2\beta})$$

$$(1 - \gamma_1)e^{(k-2)\beta} + \gamma_1(1 - e^{-2\beta}) \leq 1$$

$$\gamma_1(1 - e^{-\beta}) + \gamma_2(e^{(k-1)\beta} - e^{(k-2)\beta}) \leq -\beta \lambda / 2$$

Using our restrictions on the structure of $R$, the above inequalities imply

$$\Delta_t \leq (1 - \gamma_1)e^{(k-2)\beta} + (1 - \rho)\gamma_1(1 - e^{-2\beta}) + \rho \left( \gamma_1(e^{-\beta} - e^{-2\beta}) + \gamma_2(e^{(k-1)\beta} - e^{(k-2)\beta}) \right)$$

$$= (1 - \gamma_1)e^{(k-2)\beta} + \gamma_1(1 - e^{-2\beta}) + \rho \left( \gamma_1(1 - e^{-\beta}) + \gamma_2(e^{(k-1)\beta} - e^{(k-2)\beta}) \right)$$

$$\leq 1 + \rho \left( \gamma_1(1 - e^{-\beta}) + \gamma_2(e^{(k-1)\beta} - e^{(k-2)\beta}) \right)$$

$$\leq 1 - \rho \lambda \beta / 2$$

\[\square\]

**B.2. Proof of Lemma 4**

**Lemma 4.** Pick $k \geq 1$. Suppose Assumption 2 holds and $\beta \leq \lambda / k$. Then for any query $a_t$, we have

$$\mathbb{E} \left[ \frac{1}{\pi_t(g^*)^k} \mid \mathcal{F}_{t-1}, a_t \right] \leq \frac{1}{\pi_{t-1}(g^*)^k}.$$

**Proof.** Suppose we query $a$ at step $t$. Denote by $\gamma_i = \eta(y_i | a)$ and $\pi_i = \pi_{t-1}(G_{0i}^*)$, and assume w.l.o.g that $g^*(a) = y_1$ and $\gamma_1 > \gamma_2 \geq \gamma_3 \geq \cdots$. Then we have

$$\mathbb{E} \left[ \frac{1}{\pi_t(g^*)^k} \mid \pi_{t-1}(g^*) \right] = \frac{\gamma_1 \pi_1 + e^{-\beta}(1 - \pi_1)^k}{\pi_{t-1}(g^*)^k} + \sum_{i \geq 2} \frac{\gamma_i(e^\beta \pi_i + 1 - \pi_i)^k}{\pi_{t-1}(g^*)^k}$$

$$= \frac{1}{\pi_{t-1}(g^*)^k} \left( \gamma_1 \pi_1 + e^{-\beta}(1 - \pi_1)^k + \sum_{i \geq 2} \gamma_i(e^\beta \pi_i + 1 - \pi_i)^k \right)$$
Denote the term in parenthesis by $\Delta_t$. Using the inequalities $1 + x \leq e^x \leq 1 + x + x^2$ for $|x| \leq 1$, for our choice of $\beta$ we have

$$\Delta_t \leq \gamma_1(\pi_1 + (1 - \beta + \beta^2)(1 - \pi_1))^k + \sum_{i \geq 2} \gamma_i((1 + \beta + \beta^2)\pi_i + 1 - \pi_i)^k$$

$$= \gamma_1(1 - \beta(1 - \beta)(1 - \pi_1))^k + \sum_{i \geq 2} \gamma_i(1 + \pi_i \beta(1 + \beta))^k$$

$$\leq \gamma_1 \exp(-k \beta(1 - \beta)(1 - \pi_1)) + \sum_{i \geq 2} \gamma_i \exp(k \pi_i \beta(1 + \beta))$$

$$\leq \gamma_1(1 - k \beta(1 - \beta)(1 - \pi_1) + (k \beta(1 - \beta)(1 - \pi_1))^2 + \sum_{i \geq 2} \gamma_i(1 + k \pi_i \beta(1 + \beta) + (k \pi_i \beta(1 + \beta))^2)$$

$$\leq 1 + k \beta \sum_{i \geq 2} \gamma_i \pi_i - \gamma_1(1 - \beta(1 - \pi_1)) + k^2 \beta^2 \sum_{i \geq 2} \gamma_i \pi_i^2 + \gamma_1(1 - \beta)^2(1 - \pi_1)^2$$

$$\leq 1 + k \beta(1 - \pi_1)(\gamma_2(1 + \beta) - \gamma_1(1 - \beta)) + k^2 \beta^2(1 - \pi_1)^2 (\gamma_2(1 + \beta)^2 + \gamma_1(1 - \beta)^2)$$

$$= 1 + k \beta(1 - \pi_1)(\beta(\gamma_1 + \gamma_2)(1 + k(1 - \pi_1) + \beta^2 k(1 - \pi_1)) - (\gamma_1 - \gamma_2)(1 + 2 \beta^2 k(1 - \pi_1))$$

$$\leq 1 + k \beta(1 - \pi_1)(\beta k - \lambda) \leq 1.$$

\[\Box\]

**B.3. Proof of Theorem 9**

For a round $t$, let $V_t$ denote the version space, i.e. the set of structures consistent with the responses seen so far. Then we may write

$$\pi_t(g) = \frac{\pi(g)\mathbb{1}[g \in V_t]}{\pi(V_t)} \quad \text{and} \quad \nu_t(g) = \frac{\nu(g)\mathbb{1}[g \in V_t]}{\nu(V_t)}.$$  

Assumption 3 tells us that we have the following upper bound.

$$D(\pi_t, \nu_t) \leq \lambda^2 \text{avg-diam}(\pi_t).$$

Thus, the average diameter of $\text{avg-diam}(\pi_t)$ is a meaningful surrogate for the objective $D(\pi_t, \nu_t)$ in this setting. Moreover, as the following lemma shows, we can estimate $\text{avg-diam}(\pi_t)$ using samples from $\pi_t$, allowing us to decide when to stop.

**Lemma 11.** Pick $\epsilon, \delta > 0$ and let $n_t = \frac{48}{\epsilon^2} \log \frac{\pi^2 \nu^2}{\delta^4}$. If at the beginning of each round $t$, we draw $E = \{\{h_1, h'_1\}, \ldots, \{h_{n_t}, h'_{n_t}\}\} \sim \pi_t$, then with probability $1 - \delta$

$$\frac{1}{n_t} \psi(E) > \frac{3\epsilon}{4} \quad \text{if} \quad \text{avg-diam}(\pi_t) > \epsilon$$

$$\frac{1}{n_t} \psi(E) \leq \frac{3\epsilon}{4} \quad \text{if} \quad \text{avg-diam}(\pi_t) \leq \epsilon/2$$

for all rounds $t \geq 1$.

The proof of Lemma 11 follows from applying a union bound to Lemma 7 of (Tosh & Dasgupta, 2017).

Recalling the definition of average splitting, we know that if we always query points that $\rho$-average the current posterior, then after $t$ rounds we will have

$$\pi(V_t)\text{avg-diam}(\pi_t) \leq (1 - \rho)^t \pi(V_0)\text{avg-diam}(\pi) \leq e^{-\rho t}.$$  

While this demonstrates that the potential function $\pi(V_t)\text{avg-diam}(\pi_t)$ is decreasing exponentially quickly, it does not by itself guarantee that $\text{avg-diam}(\pi_t)$ is itself decreasing. What is needed is a lower bound on the factor $\pi(V_t)$. The following lemma, which is a generalization of a result due to Freund et al. (1997), provides us with just that, provided that $G$ has bounded graph dimension.

**Lemma 12.** Suppose $g^* \sim \nu$ where $\nu$ is a prior distribution over a hypothesis class $G$ with graph dimension $d_G$, and say $|Y| \leq k$. Let $c > 0$ and $a_1, \ldots, a_m$ be any atomic questions, and let $V^* = \{g \in G : g(a_i) = g^*(a_i) \text{ for all } i\}$, then

$$\Pr \left( \log \left( \frac{1}{\nu(V^*)} \right) \geq c + d_G \log \frac{em(k + 1)}{d_G} \right) \leq e^{-c}.$$
To prove this, we need the following generalization of Sauer’s lemma.

**Lemma 13** (Corollary 3 of [Haussler & Long, 1995]). Let \( d, m, k \) be s.t. \( d \leq m \). Let \( F \subset \{1, \ldots, k\}^m \) s.t. \( F \) has graph dimension less than \( d \). Then,

\[
|F| \leq \sum_{i=0}^{d} \binom{m}{i}(k+1)^i \leq \left( \frac{em(k + 1)}{d} \right)^d.
\]

**Proof of Lemma 12.** Let \( V_1, \ldots, V_N \subset G \) denote the partition of \( G \) induced by our atomic questions. Note that if \( g^* \sim \nu \), then the probability \( V^* = V_i \) is exactly \( \nu(V_i) \). Let \( S \subset \{1, \ldots, N\} \) consist of all indices \( i \) satisfying \( \log \frac{1}{\nu(V_i)} \geq \epsilon + \log N \).

Rearranging, we have

\[
\sum_{i \in S} \nu(V_i) \leq 2^{-c} \cdot \left| S \right| \leq 2^{-c}.
\]

From Lemma 13, we have \( \log N \leq d_G \log \frac{em(k + 1)}{d_G} \), which finishes the proof.

Given the above, we are now ready to prove Theorem 9.

**Theorem 9.** Suppose \( G \) has average splitting index \( (\rho, \epsilon/(2\lambda^2), \tau) \) and graph dimension \( d_G \). If Assumption 3 holds and the noise rate is zero then with probability \( 1 - \delta \), NDBAL terminates with a distribution \( \pi_t \) satisfying \( D(\pi_t, \nu_t) \leq \epsilon \) while using the following resources:

1. \( T \leq O \left( \frac{d_G \log \frac{|Y| |J|}{\epsilon \tau \log 2}}{\rho} \right) \) rounds with one label per round,
2. \( m_t \leq \frac{1}{\tau} \log \frac{\epsilon^2 \pi^2}{3\delta} \) unlabeled data points drawn per round, and
3. \( n \leq O \left( \frac{1}{\epsilon \rho} \log \frac{(m + |Y|)T}{\delta} \right) \) structures sampled per round.

**Proof.** If we use the stopping criterion from Lemma 11 with the threshold \( 3\epsilon/4\lambda^2 \), then at the expense of drawing an extra \( O \left( \frac{d_G^2 \log \frac{d_G^2}{\rho \delta}}{\rho} \right) \) hypotheses per round \( t \), we are guaranteed that with high probability if we ever encounter a round \( t \) in which \( \text{avg-diam}(\pi_t) \leq \epsilon/(2\lambda^2) \) then we terminate and we also never terminate whenever \( \text{avg-diam}(\pi_K) > \epsilon \). Thus if we do ever terminate at some round \( t \), then with high probability

\[
D(\pi_t, \nu_t) \leq \lambda^2 \text{avg-diam}(\pi_t) \leq \epsilon.
\]

Thus, it remains to be shown that we will encounter such a posterior. Note that if we draw \( m_t \geq \frac{1}{\tau} \log \frac{\epsilon^2 \pi^2}{3\delta} \) unlabeled points per round, then with high probability one of them will \( \rho \)-average split \( \pi_t \) if \( \text{avg-diam}(\pi_t) > \epsilon/(2\lambda^2) \). Conditioned on this happening, Lemma 2 guarantees that that with high probability SELECT finds a point that \( \rho/8 \)-average splits \( \pi_t \).

If after \( T \) rounds we still have not terminated, then \( \text{avg-diam}(\pi_T) > \epsilon/(2\lambda^2) \). However, we also know

\[
\pi(V_T)^2 \text{avg-diam}(\pi_T) \leq e^{-\rho T/8}.
\]

Now suppose that in each round \( t \), we have seen \( m_t \) unlabeled data points \( x_1^{(t)}, \ldots, x_{m_t}^{(t)} \), and define \( V_{T_t} = \{ h \in H : h(x_1^{(t)}) = h^*(x_1^{(t)}) \} \) for \( t = 1, \ldots, T, i = 1, \ldots, m_t \). Then clearly, \( V_{T_t} \subset V_T \). By Lemma 12, we have with probability \( 1 - \delta/2 \),

\[
\pi(V_T) \geq \pi(V_{T_t}) \geq \frac{1}{\lambda} \nu(V_{T_t}) \geq \frac{1}{\lambda} \cdot \frac{3\delta}{\pi^2 T^2} \left( \frac{d_G}{em(k + 1)} \right)^{d_G}
\]

for all rounds \( T \geq 1 \).

Plugging this in with the above, we have

\[
\text{avg-diam}(\pi_T) \leq \frac{e^{-\rho T/8}}{\pi(V_T)^2} \leq \lambda^2 \exp \left( 2d_G \log \frac{em(k + 1)}{d_G} + 2 \log \frac{\pi^2 T^2}{3\delta} - \frac{\rho T}{8} \right).
\]
Note that we can upper bound $m$ as

$$m \leq \sum_{t=1}^{T} m_t \leq \frac{T \log T^2 \pi^2}{3\delta}.$$

Putting everything together, we have

$$\frac{\epsilon}{\lambda^2} \leq \text{avg-diam}(\pi_T) \leq \lambda^2 \exp \left( 2 \log \frac{\pi^2 T^2}{3\delta} + 2d_G \log \left( \frac{\epsilon(k + 1)}{d_G} \cdot \frac{T \log T^2 \pi^2}{3\delta} \right) - \frac{\rho T}{8} \right).$$

Letting $C = 2d_G \log \frac{\epsilon(k + 1)}{\rho \tau}$ and $b = \frac{\pi^2}{3\delta}$, the right-hand side is less than $\epsilon/(2\lambda^2)$, whenever

$$T \geq \frac{8}{\rho} \max \left\{ C + \log \frac{2\lambda^4}{\epsilon} + 6(d + 1) \log T, C + \log \frac{2\lambda^4}{\epsilon} + \log b + 2d \log (3b \log(b)) \right\}.$$

Additionally, note that $T \leq \frac{8}{\rho} \left( C + \log \frac{1}{\rho} + 6(d + 1) \log T \right)$, whenever

$$T \geq \frac{16}{\rho} \max \left\{ C + \log \frac{2\lambda^4}{\epsilon}, 24(d + 1) \log^2 \left( \frac{96(d_G + 1)}{\rho} \right) \right\}.$$

The value of $T$ provided in the theorem statement, satisfies all of these inequalities. Thus, with high probability, we must have encountered a round in which $\text{avg-diam}(\pi_t) < \epsilon/(2\lambda^2)$ and terminated.