Active Learning for Regression and Classification
by Inverse Distance Weighting

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Abstract

This paper proposes an active learning algorithm for solving regression and clas-
sification problems based on inverse-distance weighting functions for selecting the
feature vectors to query. The algorithm has the following features: (i) supports
both pool-based and population-based sampling; (ii) is independent of the type of
predictor used; (iii) can handle known and unknown constraints on the queryable
feature vectors; and (iv) can run either sequentially, or in batch mode, depending on
how often the predictor is retrained. The method’s potential is shown in numerical
tests on illustrative synthetic problems and real-world regression and classification
datasets from the UCI repository. A Python implementation of the algorithm that we
call IDEAL (Inverse-Distance based Exploration for Active Learning), is available at
http://cse.lab.imtlucca.it/~bemporad/ideal

Keywords: Active learning (AL), inverse distance weighting, pool-based sampling, query
synthesis, supervised learning, regression, classification, neural networks.

1 Introduction

Active learning (AL) strategies are used in supervised learning to let the training algorithm
“ask questions” [1], i.e., choose the feature vectors to query for the corresponding target
value during the training phase based on the model learned so far. The main aim of AL
is to possibly reduce the number of training samples required to train the model, or in
other words, to get a model of the same prediction quality with a smaller dataset. This
is particularly useful when knowing the target value associated with a given combination
of features is an expensive operation, for example, it may involve asking a human to
“label” samples manually, running a costly and time-consuming laboratory experiment,
or performing a complex computer simulation.

AL methods are usually categorized in query synthesis (or population-based) meth-
ods, in which the feature vector to query can be chosen arbitrarily, pool-based sampling
methods, in which the vector can only be chosen within a given finite set (or “pool”) of
unlabeled values, and selective-sampling methods, in which vectors are proposed in
a streaming flow, and the AL algorithm can only decide online whether to ask for the
Corresponding target or not [1].

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Several approaches to AL are available in the literature, see, e.g., the survey papers [1–5]. Most of the literature focuses on classification problems [4,6], although AL has also been investigated for regression [7–10] and clustering. We refer to the recent survey paper [5] for a detailed and updated taxonomy of AL methods for classification, regression, and clustering.

As pointed out in [10], AL methods should collect data that are informative, representative, and diverse, i.e., respectively, contain rich information for reducing modeling errors, cover portions of the feature vector space where the predictor is evaluated most frequently and in particular reject outliers, and explore such a space trying to avoid sampling the same regions too often. AL methods are often linked to a specific class of predictors, such as neural networks [7] or mixtures of Gaussians and locally weighted regression [8], or to a particular learning algorithm [9]. Moreover, AL methods are typically computationally involved in the case optimal sampling is sought, or in query-by-committee methods [11] in which multiple predictors need to be trained to measure their disagreement.

AL is related to the problem of optimally designing experiments, whose origin dates back at least to the 30s [12], and has attracted an extensive literature for decades [13]. Another problem related to AL is black-box derivative-free optimization [14] in which a surrogate of the objective function is learned incrementally from a finite number of samples of it, such as in Bayesian optimization methods [15]. Compared to solving a supervised learning problem, where the objective is to find a model that reproduces well the underlying process over the entire set of feature-vectors of interest, in black-box optimization the problem is somehow simpler, as the interest is limited to approximating the objective function well around one of its global minimizers.

1.1 Contribution

In this paper, we provide a unified AL framework for regression and classification that is entirely independent of the particular predictor function used, that can address both pool-based and population-based settings, and is not computationally involved. By leveraging on ideas we previously investigated for global optimization based on surrogate functions [16], we propose an AL method in which the uncertainty associated with the currently available predictor and the exploration function used to sample the feature-vector space are characterized by inverse-distance weighting (IDW) functions.

The proposed algorithm that we call IDEAL (Inverse-Distance based Exploration for Active Learning) blends different requirements: informativeness, by sampling feature-vector regions where model uncertainty is estimated to be larger; representativeness, in the case of pool-based sampling, by taking into account a density function similar to the one used in density-based spatial clustering approaches [17]; and diversity, using an IDW exploration term that is higher far away from samples that have already been queried. The algorithm can also handle constraints on the feature vectors that can be queried, that can either be known a priori or even unknown. The latter case covers the situation in which one discovers only after querying certain combinations of features that the corresponding target cannot be retrieved, for example, because a specific physical experiment cannot be performed or a computer simulation does not converge. Finally, the proposed algorithm can be run either sequentially, by retraining the predictor after each successful query, or in batch mode, by retraining only after querying a certain prescribed finite number of samples.

The paper is organized as follows. After formulating the AL problem in Section 2, we
describe the proposed algorithm in Section 3. Numerical tests on synthetic and real-world regression and classification problems are reported in Section 4 and some conclusions are drawn in Section 5.

2 Active learning problem

We consider a process \( y : \mathcal{X} \to \mathcal{Y} \) generating data \( y_k = y(x_k) \), where \( \mathcal{X} \subseteq \mathbb{R}^n \) is the set of feature vectors, \( x_k \in \mathcal{X} \), and \( \mathcal{Y} \subseteq \mathbb{R}^m \) is the set of corresponding targets \( y_k, y_k \in \mathcal{Y} \). As the process \( y \) is unknown, we wish to find a predictor \( \hat{y} : \mathcal{X} \to \mathcal{Y} \) solving the supervised learning problem

\[
\min_y \int_{\mathcal{X} \cap \mathcal{X}} \ell(y(x), \hat{y}(x), x) dx
\]

where \( \ell : \mathcal{Y} \times \mathcal{Y} \times \mathcal{X} \to \mathbb{R} \) is a loss function and \( \mathcal{X} \subseteq \mathbb{R}^n \) is a bounded set of feature vectors \( x \) of interest, i.e., for which we want to obtain a good approximation \( \hat{y}(x) \) of \( y(x) \). While the set \( \mathcal{X} \) is known, for example, it may be defined by the set of inequality constraints

\[
\mathcal{X} = \{ x : \mathbb{R}^n : g_i(x) \leq 0, \ i = 1, \ldots, n_c \}
\]

g \in \mathbb{R}^n \to \mathbb{R} \), the set \( \mathcal{X} \) for which \( y(x) \) is defined could be unknown, as we might not be able to know a priori whether for a given \( x \in \mathcal{X} \) its corresponding target \( y(x) \) can be obtained. For example, evaluating \( y(x) \) may require running a complex experiment or computer simulation, and this could not be completed for various reasons. In such cases, characterizing the shape of \( \mathcal{X} \), if of interest, would be a binary classification problem itself that is amenable to active learning. Note that in the case of multiple targets \( m > 1 \), we could generalize the setting by assuming that each process component \( [y]_i : \mathcal{X}_i \to \mathcal{Y}_i, \ i = 1, \ldots, m \). However, for simplicity of notation, we assume here that \( \mathcal{X} = \cap_{i=1}^m \mathcal{X}_i \), i.e., that either the entire output vector \( y(x) \) is defined or it is entirely undefined at a given \( x \).

Special cases of (1) are (multivariate) regression problems (\( \mathcal{Y} = \mathbb{R}^m \)) and classification problems (\( \mathcal{Y} = \{0, 1\}^m \)). We assume that possible discrete features have been one-hot encoded, and that hence in general \( \mathcal{X} \subseteq \{0, 1\}^{n_b} \times \mathbb{R}^{n_n} \), where \( n_b \) and \( n_n \) are the number of binary and numeric features, respectively, \( n = n_b + n_n \), and that the loss \( \ell \) contains impulsive terms (Dirac delta terms) so that (1) can be rewritten as

\[
\min_y \sum_{x_b \in \mathcal{X}_b \cap \mathcal{X}_c} \int_{\mathcal{X}_c \cap \mathcal{X}_c} \ell(y(x), \hat{y}(x), x_c, x_b) dx_c
\]

where \( x_b \) denotes the subvector of binary components of the feature vector \( x \), \( \mathcal{X}_b (\mathcal{X}_c) \) the corresponding set of their admissible combinations (of interest), and \( \mathcal{X}_c (\mathcal{X}_c) \) the set of admissible subvectors \( x_c \) of numeric features (of interest).

In order to address problem (1), we will solve its empirical approximation

\[
\min_y \frac{1}{N} \sum_{k=1}^N \ell(y_k, \hat{y}(x_k), x_k)
\]

where \( D_N \triangleq \{(x_k, y_k)\}_{k=1}^N \) is a training dataset, with \( y_k = y(x_k) \) \( ^1 \)

\( ^1 \)Although function \( y \) is rather arbitrary, the formulation could be extended to explicitly include a noise term \( \eta_n \in \mathbb{R}^n \), so that \( y_k = y(x_k, \eta_k) \) is available rather than \( y(x_k) \). This would allow modeling non-reproducible queries, i.e., \( y_k \neq y_j \) for \( x_k = x_j, k \neq j \).
In (supervised) passive learning the training dataset \( D_\mathcal{X} \) is given, where clearly \( x_k \in \mathcal{X} \) for all \( k = 1, \ldots, N \), as the corresponding targets \( y_k \) have been acquired. Instead, in active learning we are free to select the training vectors \( x_k \) to query, i.e., for which we want to get the corresponding target value \( y_k \), if it is defined, or a declaration that \( x_k \notin \mathcal{X} \). We have a pool-based AL problem when \( x_k \) can only be selected from a pool \( \mathcal{X}_P = \{ \bar{x}_j \}_{j=1}^M \) of samples, \( M \geq N \), with \( \mathcal{X}_P \subseteq \bar{\mathcal{X}} \), or a population-based AL problem when \( x_k \) can be chosen freely within the given bounded set \( \mathcal{X}_P = \bar{\mathcal{X}} \).

3 Active learning algorithm

Let \([x_{\min}, x_{\max}] \subset \mathbb{R}^n\) be the smallest hyper-box containing the feature vectors we are allowed to sample, i.e.,

\[
[x_{\min}]_i \triangleq \min_{x \in \mathcal{X}_P} [x]_i, \quad [x_{\max}]_i \triangleq \max_{x \in \mathcal{X}_P} [x]_i,
\]

which in case of pool-based AL is equivalent to setting

\[
[x_{\min}]_i \triangleq \min_{j=1, \ldots, M} [\bar{x}]_j, \quad [x_{\max}]_i \triangleq \max_{j=1, \ldots, M} [\bar{x}]_j
\]

(4b)

In order to be immune to different scaling of the individual features, when querying samples we consider the scaling function \( s : \mathbb{R}^n \to \mathbb{R}^n \) defined by

\[
\sigma(x) \triangleq \text{diag} \left( \frac{2}{x_{\max} - x_{\min}} \right) \left( x - \frac{x_{\max} + x_{\min}}{2} \right)
\]

(4c)

where clearly \( \sigma(x) \in [-1, 1]^n \) for all \( x \in [x_{\min}, x_{\max}] \).

Let \( N_{\text{max}} \) be the total budget of queries we have available to perform the AL task. During AL, we keep track of samples \( x_k \) that have been selected and for which the corresponding target could be acquired in the set \( Q \subseteq \{1, \ldots, N_{\text{max}}\} \) of indices\(^2\) i.e., \( k \in Q \) if and only if \( x_k \in \mathcal{X} \). Moreover, in the case of pool-based sampling, we keep track in the set \( \mathcal{E} \subseteq \{1, \ldots, M\} \) of the indices of samples already extracted from the pool \( \mathcal{X}_P \) that have been tested, to avoid possibly querying them again.

3.1 Initialization

Before fitting any prediction model, as commonly done in most AL approaches, we must first select \( N_i \) samples \( x_1, \ldots, x_{N_i} \in \bar{\mathcal{X}} \cap \mathcal{X} \). In case of population-based AL, we use Latin Hypercube Sampling (LHS)\(^{18}\) on the hyper-box \([x_{\min}, x_{\max}]\); in the case of pool-based AL, we run instead the K-means algorithm\(^{19}\) on the pool \( \mathcal{X}_P^\sigma \triangleq \sigma(\mathcal{X}_P) \) of scaled samples with \( K = N_i \) and pickup the \( N_i \) different vectors \( \sigma(\bar{x}_1), \ldots, \sigma(\bar{x}_{N_i}) \in \mathcal{X}_P^\sigma \) that are closest to the centroids obtained by K-means in terms of Euclidean distance (cf.\(^{10}\)). As some vectors may be infeasible (\( \bar{x}_k \notin \bar{\mathcal{X}} \)) or cannot be queried (\( \bar{x}_k \notin \mathcal{X} \)), similarly to the LHS algorithm with constraints described in\(^{16}\) Algorithm 2) the vectors \( \bar{x}_k \notin \bar{\mathcal{X}} \cap \mathcal{X} \) are discarded, and the above procedure is repeated until a set of \( N_i \) pairs \( (\bar{x}_k, y_k) \) is collected.

We denote by \( N_{\text{init}} \), \( N_{\text{init}} \geq N_i \), the total number of samples queried during the initialization phase and by \( \{(x_i, y_i)\}, i = 1, \ldots, N_i \) the resulting set of collected samples.

\(^{2}\)In case of multiple targets \( m > 1 \) and different feasible sets \( \mathcal{X}_i \), i.e., \( [y_i] : \mathcal{X}_i \to \mathcal{Y}_i \), one could define a separate set \( Q_i \) for each target \( i = 1, \ldots, m \), with \( k \in Q_i \) if and only if \( x_k \in \mathcal{X}_i \).
Note that in the case \( X \subset \bar{X}, \) \( N_{\text{init}} > N_{i} \) queries might be required to get \( N_{i} \) pairs \((x_{k}, y_{k})\), as samples \( x \in \bar{X} \setminus X \) might be encountered for which \( y(x) \) is not defined. In this case, \( N_{\text{init}} \in Q \), as the initialization phase terminates as long as \( N_{i} \) pairs have been successfully collected. Note also that in case \( N_{i} \) valid samples cannot be retrieved at initialization within the total budget \( N_{\text{max}} \) of queries we have available, the AL task cannot proceed further.

### 3.2 Query-point selection

Assume that we have collected \( N \) samples \( x_{k} \) and, \( \forall k \in Q \), the corresponding target values \( y_{k} \), and that we have fit a predictor \( \hat{y}(x) \) on them by solving the supervised learning problem as in (3)

\[
\hat{y} = \arg \min_{\hat{y}} \sum_{k \in Q} \ell(y_{k}, \hat{y}(x_{k}), x_{k}) \tag{5}
\]

Note that (5) is a regression problem in the case all targets are numeric \((y_{k} \in \mathbb{R}^{m})\), or a classification problem when \( y_{k} \in \{0, 1\}^{m} \), or a mix of the two when \( m > 1 \) and both numeric and binary targets are present.

Then, we need to define a criterion to select the remaining \( N_{\text{max}} - N_{\text{init}} \) samples \( x_{k} \) to query. In this paper, we will select the next sample \( x_{N+1} \) to query by maximizing an acquisition function \( a : \mathbb{R}^{n} \to [0, +\infty) \) that we will introduce in the sequel

\[
x_{N+1} = \arg \max_{x \in \mathcal{X}} a(x) \tag{6}
\]

retrain \( \hat{y}(x) \) if \( y(x_{N+1}) \) is defined (i.e., if \( x_{N+1} \in \mathcal{X} \)), update the acquisition function \( a \), increase \( N \), and so on, until \( N = N_{\text{max}} \) and the total available budget for queries is exhausted. The approach can be extended easily to batch-mode active learning by retraining \( \hat{y}(x) \) only after \( T \) new queries have been performed, \( T > 1 \).

To define the acquisition function \( a \), we want to use an empirical estimation of the uncertainty \( s_{i}(x) \), \( s_{i} : \mathbb{R}^{n} \to [0, +\infty) \), associated with each component \( i \) of the prediction \( \hat{y}(x) \), \( i = 1, \ldots, m \), that we define here as we proposed in [16] to promote exploration in global optimization using surrogate functions.

Given a set \( \{x_{k}\}_{k=1}^{N} \) of vectors of \( \mathbb{R}^{n} \), we consider the squared (scaled) Euclidean distance function \( d^{2} : \mathbb{R}^{n} \times \mathbb{R}^{n} \to \mathbb{R} \)

\[
d^{2}(x, x_{k}) = ||\sigma(x) - \sigma(x_{k})||_{2}^{2}, i = 1, \ldots, N \tag{7}
\]

In standard IDW functions [20], the weight functions \( w_{k} : \mathbb{R}^{n} \setminus \{x_{k}\} \to \mathbb{R} \) are defined by the squared inverse distances

\[
w_{k}(x) = \frac{1}{d^{2}(x, x_{k})} \tag{8a}
\]

In order to make the weight decay more quickly as \( x \) gets more distant from \( x_{k} \), as suggested in [16][21], here we adopt the alternative weighting function

\[
w_{k}(x) = \frac{e^{-d^{2}(x, x_{k})}}{d^{2}(x, x_{k})} \tag{8b}
\]

Then, we define the following functions \( v_{k} : \mathbb{R}^{n} \to \mathbb{R} \) for \( k = 1, \ldots, N \) as

\[
v_{k}(x) = \begin{cases} 
1 & \text{if } x = x_{k} \\
0 & \text{if } x = x_{j}, j \neq k \\
\frac{w_{k}(x)}{\sum_{j=1}^{N} w_{k}(x)} & \text{otherwise}
\end{cases} \tag{9}
\]
As suggested in [16,21], we then define $s^2 : \mathbb{R}^n \to \mathbb{R}^m$ as the IDW variance function

$$s^2_i(x) = \sum_{k \in Q} v_k(x)([y_k]_i - [\hat{y}(x)]_i)^2, \ i = 1, \ldots, m$$

(10)

associated with the current training dataset $\{(x_k, y_k)\}_k^N$ and predictor $\hat{y}$. Note that for $x = x_k$ and $k \in Q$ we have $s^2_i(x_k) = ([y_k]_i - [\hat{y}(x_k)]_i)^2$, which in case of perfect interpolation $[\hat{y}(x_k)]_i = [y_k]_i$ gives $s^2_i(x_k) = 0$ (this corresponds to having no prediction uncertainty about $y_i(x)$ at $x = x_k$). Note also that the sum in (10) only considers the indices $k \in Q$, as for $k \not\in Q$ vector $x_k \not\in \mathcal{X}$ and therefore $y_k = y(x_k)$ is undefined.

**Example 3.1** Let the data $y_k$ be generated by the following scalar function $y : \mathbb{R} \to \mathbb{R}$

$$y(x) = x^4 \sin^2 \left( \frac{1}{3} x^2 \right)$$

(11)

that we want to approximate over the interval $\bar{\mathcal{X}} = [-3,3]$ by a simple feedforward NN $\hat{y}$ with two layers of five neurons each, logistic activation function $\frac{1}{1+e^{-x}}$, and linear output function. As depicted in Figure 1 we assume that we have collected $N = 7$ samples $(x_k, y_k)$ (blue dots), $y_k = y(x_k)$, and fit a NN via the `MLPRegressor` function in `scikit-learn` with $\ell_2$-regularization term $\alpha = 10^{-2}$, by using the LBFGS nonlinear optimization algorithm. Figure 1 also shows the original function $y(x)$ (blue line), the NN predictor $\hat{y}(x)$ (red line), and the band $\hat{y}(x) \pm 3\sqrt{s^2_i(x)}$ (light blue area). The figure also shows scaled and shifted versions of the IDW functions $s^2_i(x)$ (green line) and $z(x)$ (dashed gray line).

For pool-based AL, we also consider the density function $\rho : \mathcal{X}_P \to (0,+\infty)$ that measures how much “isolated” is a sample $\bar{x}_k \in \mathcal{X}_P$ with respect to the remaining samples. Similar to density-based spatial clustering approaches [17], we use the average distance of
\( \bar{x}_k \) from its \( n \) nearest neighbors,

\[
d_k = \frac{1}{n} \sum_{j \in N_k} \| \bar{x}_k - \bar{x}_j \|
\]

where \( I_k \) is the set of indices corresponding the \( n \) nearest neighbors of \( \bar{x}_k \) in \( \mathcal{X}_P \backslash \{ \bar{x}_k \} \), to estimate the density as proportional to the normalized inverse volume of the sphere of radius \( d_k \), i.e.,

\[
\rho(\bar{x}_k) = \frac{1}{\pi^{n/2}} \frac{1}{\max_{j=1,\ldots,M} \left\{ \frac{1}{\pi_j} \right\}} = \frac{\min_{j=1,\ldots,M} \left\{ d_k^n \right\}}{d_k^n} = \frac{\min_{j=1,\ldots,M} \left\{ d_k^n \right\}}{\max_{j=1,\ldots,M} \left\{ d_k^n \right\}}
\]

(12)

We assume that duplicates \( \bar{x}_k = \bar{x}_j \) have been removed, as \( n \) duplicates would result in a zero average distance and therefore make (12) undefined. Note that \( \rho \) does not depend on the predictor \( \hat{y} \) learned and can be therefore computed upfront. Regarding population-based AL, we simply set \( \rho(x) = 1, \forall x \in \mathcal{X} \).

As suggested in [16] for global optimization using surrogate functions, we also consider the IDW distance function \( z : \mathbb{R}^n \rightarrow \mathbb{R} \) defined as

\[
z(x) = \begin{cases} 0 & \text{if } x \in \{x_1, \ldots, x_N\} \\ \frac{2}{\pi} \tan^{-1} \left( \frac{1}{\sum_{k=1}^N w_k(x)} \right) & \text{otherwise} \end{cases}
\]

(13)

Similarly to the passive sampling approach in [23], function \( z \) returns a pure exploration term that is only based on the geometric position of the (scaled) feature vectors \( \{x_k\} \), and hence, contrarily to the IDW variance function \( s^2 \), does not exploit the predictor \( \hat{y} \) learned up to step \( N \). Note that \( s^2 \) also promotes exploration, but only indirectly.

Let us now define the acquisition function

\[
a(x) = (1 + \omega \rho(x)) \sum_{i=1}^m c_i(x)(s_i^2(x) + \delta z(x))
\]

(14)

where \( \delta \geq 0 \) is a hyperparameter balancing the role of IDW variance \( s^2(x) \) and IDW distance \( z(x) \), \( c_i : \mathbb{R}^n \rightarrow [0, +\infty) \) is a weight function that can be used to actively learn the predictor in a non-uniform way with respect to \( x \) (or uniformly, if \( c_i(x) \equiv 1 \)) and the target index \( i \), and \( \omega \geq 0 \) is a scalar weight on density. Note that \( \omega \) is only meaningful in case of pool-based sampling, as \( \rho(x) \equiv 1 \) when a population-based AL approach is used. Note also that \( \delta \) trades off between active learning (small \( \delta \)) and passive learning based on the pure exploration of the feature-vector space (large \( \delta \)).

In the case of population-based AL, the maximization problem [6] can be solved by global optimization; in this paper, we will use the derivative-free Particle Swarm Optimization (PSO) algorithm [24], as \( a(x) \) is a cheap function to evaluate whenever \( \hat{y}(x) \) is easy to compute. In pool-based sampling, when the number \( M \) of samples in the pool is not too high, problem (6) can be solved by enumeration:

\[
x_{N+1} = \bar{x}_{k^*}, \ k^* = \arg \min_{k \in \{1, \ldots, M\} \backslash \mathcal{E}} \{ a(\bar{x}_k) \}
\]

(15a)

When the above is impractical due to a large number \( M \) of samples in the pool one can first use PSO to optimize over the entire set \( \mathcal{X} \) to get \( \bar{x}^* = \arg \max_{x \in \mathcal{X}} a(x) \) as in population-based AL and then set (cf. [25])

\[
x_{N+1} = \bar{x}_{k^*}, \ k^* = \arg \min_{k \in \{1, \ldots, M\} \backslash \mathcal{E}} \{ \| \bar{x}_k - x^* \|_2^2 \}
\]

(15b)
Let us show that the active learning mechanism (6), (14) follows criteria of informativeness, representativeness, and diversity, which are listed in [10] as essential for AL. Regarding the first, maximizing \( a(x) \) implies looking for large values of the uncertainty \( s(x) \) associated with the current predictor \( \hat{y}(x) \), i.e., to select the next sample \( x_{N+1} \) where \( \hat{y} \) is considered most uncertain according to (10), so that querying \( x_{N+1} \) is expected to bring significant new information. The second, which is only applicable in the case of pool-based sampling, is taken care of by \( \rho(x) \) when \( \omega > 0 \), as in the maximization (6) those samples \( \bar{x}_k \) that have a low density \( \rho(\bar{x}_k) \), for instance, because they are outliers, will be discouraged. Third, diversity is promoted because \( s(x) \) and \( z(x) \) are small close to samples that have been already visited, which ultimately makes the AL algorithm visit unexplored areas of the feature-vector space. The tradeoff between representativeness and diversity is taken care of by the coefficient \( \omega \).

Algorithm 1 reports the pseudocode of the proposed AL algorithm that we call Inverse-Distance based Exploration for Active Learning (IDEAL). The main complexity of Algorithm 1 is due to retraining the predictor \( \hat{y} \) at Step 6.1 to exploit the new sample \( (x_{N+1}, y(x_{N+1})) \), and to solving the optimization problem at Step 6.2 to get such a sample. Regarding the former, warm-starting or incremental learning could be exploited if supported by the training algorithm. Note that output data scaling can be updated before retraining \( \hat{y} \), such as by applying standard scaling based on the currently available values \( y_k, k \in Q \). Regarding Step 6.2, the computation complexity mainly depends on the number of operations required to evaluate the predictor \( \hat{y}(x) \) in (10).

4 Numerical tests

In this section, we test the proposed AL approach on synthetic illustrative examples and real-world datasets. All computations were carried out in Python 3.8.10 on an Intel Core i9-10885H CPU @2.40GHz machine using the scikit-learn package [22] to train feedforward NNs for regression (MLPRegressor function) and classification (MLPClassifier function).

The IDEAL algorithm is compared to random sampling (random), in which samples \( x_{N+1} \) are drawn from the uniform distribution defined over \( \bar{X} \) (population-based sampling), or by selecting a random index in \( \{1, \ldots, N_{\text{max}}\} \setminus \mathcal{E} \) (pool-based sampling), and the sampling technique proposed in [23] (greedy), where \( x_{N+1} \) is selected instead by maximizing the minimum distance from existing samples, i.e.,

\[
x_{N+1} = \arg \max_{x \in X^P} \left\{ \min_{k=1, \ldots, N} \| \sigma(x) - \sigma(x_k) \|_2^2 \right\}
\]

For fair comparison, in this case the first \( N_i \) samples are also chosen as in Step 2 of Algorithm 1.

4.1 Scalar example

We first test the proposed AL approach on the simple regression problem defined in Example 3.1, i.e., with \( y \) as in (11). Since \( n = 1 \), we generated a grid \( X^P \) by collecting \( M = 1000 \) equally-spaced points on the line segment \( \hat{X} = [-3, 3] \) and use pool-based sampling, so that problem (6) can be solved by enumeration. While training the NN, the parameter vector is not warm-started when executing Step 6.1 to avoid possible low-quality local minima due to the early steps of Algorithm 1 when only a few data are available.
Algorithm 1 Inverse-Distance based Exploration for Active Learning (IDEAL).

**Input**: Set \( \mathcal{X}_P = \{ \bar{x}_k \}_{k=1}^M \) (pool-based) or \( \mathcal{X}_P = \mathcal{X} \) (population-based) of queryable feature vectors; budget \( N_{\text{max}} \) of available queries; number \( N_i \) of initial samples to acquire; pure exploration hyperparameter \( \delta \geq 0 \); density weight \( \omega \geq 0 \) (pool-based only); weight functions \( c_i, i = 1, \ldots, m \).

1. Compute scaling functions \( \sigma_i \) as in (4);
2. Extract \( N_i \) samples \( (x_k, y_k) \) as described in Section 3.1 by K-means (pool-based) or LHS (population-based); if not possible to extract within \( N_{\text{max}} \) queries go to Step 7 otherwise set \( N_{\text{init}} \) = number of queries done;
3. \( Q \leftarrow \{ k \in \{1, \ldots, N_{\text{init}} \} : x_k \in \mathcal{X} \} \);
4. \( E \leftarrow \{ i \in \{1, \ldots, M \} : \bar{x}_i = x_k \text{ for some } k \in \{1, \ldots, N_{\text{init}} \} \} \) (pool-based only);
5. Compute densities \( \{ \rho_k \} \) as in (12), \( \forall k \in \{1, \ldots, M \} \setminus E \) (pool-based only);
6. For \( N = N_{\text{init}}, \ldots, N_{\text{max}} \) do:
   6.1. If \( N \notin Q \) then update predictor \( \hat{y} \) by solving (3);
   6.2. Acquire new sample \( x_{N+1} \) as in (6) (population-based) or (15) (pool-based);
   6.3. If \( x_{N+1} \in \mathcal{X} \) get \( y_{N+1} \) and set \( Q \leftarrow Q \cup \{ N + 1 \} \);
   6.4. \( E \leftarrow E \cup \{ k^* \} \) (pool-based only);
7. End.

**Output**: Predictor \( \hat{y} \), or declaration of failure in collecting \( N_i \) feasible initial samples.

The median over 50 runs of the root-mean-square error (RMSE)

\[
RMSE = \sqrt{\frac{1}{N} \sum_{k=1}^{N} (y_k - \hat{y}(x_k))^2}
\]

obtained with \( \delta = 0, \omega = 0, c(x) \equiv 1, N_i = 4, N_{\text{max}} = 30 \), as a function of the number \( N \) of acquired samples, is depicted in Figure 2 and compared with the median RMSE obtained with random and greedy sampling. Table 1 shows the median RMSE obtained when \( N = N_{\text{max}} \) for different values of \( \delta \).

| \( \delta \) | 0   | 0.1 | 0.5 | 1.0 | 5.0  | 10.0 | G  | R  |
|----------|-----|-----|-----|-----|------|------|----|----|
|          | 0.384 | 0.388 | 0.388 | 0.392 | 0.391 | 0.396 | 0.683 | 1.366 |

Table 1: AL of function (11): median RMSE after \( N_{\text{max}} = 30 \) steps for different values of \( \delta \) (G = greedy, R = random)

In order to test robustness against measurement noise, the same experiment is repeated for \( \delta = 0 \) by perturbing the measurements \( y_k = y(x_k) + \eta_k \), where \( \eta_k \sim N(0, \sigma^2) \) for different values of the standard deviation \( \sigma \). The resulting median RMSE over 50 runs after \( N_{\text{max}} = 30 \) IDEAL iterations is shown in Table 2.
Figure 2: AL of function (11): median RMSE as a function of the number of queries

\[ \begin{array}{cccc}
\sigma_\eta & \text{IDEAL} & G & R \\
0.0 & 0.384 & 0.683 & 1.366 \\
1.0 & 0.611 & 0.799 & 1.459 \\
2.0 & 0.826 & 0.947 & 1.426 \\
\end{array} \]

Table 2: AL of function (11) with noise: median RMSE after \( N_{\text{max}} = 30 \) steps for different values of \( \sigma_\eta \) (\( G = \text{greedy}, \ R = \text{random} \))

4.2 Multiparametric quadratic programming

Model predictive control (MPC) is a popular engineering technique for controlling dynamical systems in an optimal way under operating constraints. Evaluating the MPC law requires solving a quadratic programming (QP) problem of the form

\[ z^*(x) = \arg \min_{z} \frac{1}{2} z'Qz + x'F'z \]

s.t. \( Az \leq b + Sx \)

\[ \ell \leq z \leq u \]

\[ y(x) = [I_m \ 0 \ \ldots \ 0]z^*(x) \] (17)

where \( z \in \mathbb{R}^{n_z} \) is a vector of future control moves, \( n_z \geq m \), and \( x \in \mathbb{R}^n \) is a vector of parameters that change at run time, such as estimated states and reference signals, and the Hessian matrix \( Q = Q' > 0 \). To alleviate the effort of solving (17) online for each given vector \( x \), multiparametric QP (mpQP) was proposed in [26], showing that the solution \( z^* : \mathbb{R}^n \rightarrow \mathbb{R}^{n_z} \), and therefore \( y(x) \), is continuous and piecewise affine over a polyhedral partition of a convex polyhedron \( X \subseteq \mathbb{R}^n \). The main drawback of such an explicit form of MPC is that the number of polyhedral cells tends to grow exponentially with the number of constraints in (17).

Suboptimal methods were proposed to approximate \( y(x) \), such as via NN’s [27, 28]. In order to find an approximation \( \hat{y}(x) \) of \( y(x) \), one must collect a training dataset of pairs...
Figure 3: mpQP problem ($m = 2$): median RMSE as a function of the number of queries $(x_k, y_k)$, where evaluating $y_k = y(x_k)$ requires solving a QP problem as in [17]. Randomly sampling a given set $\mathcal{X} \subset \mathbb{R}^n$ of parameters $x$ may result time-consuming, especially when the dimension $n$ of the parameter vector is large. To minimize the number $N_{\text{max}}$ of QP problems solved to get a proper approximation quality, we use Algorithm 1 to actively generate samples $x_k$.

We consider a mpQP problem with $n = 2$, $n_z = 12$, $m = 1$, $b \in \mathbb{R}^{12}$, $S = 0$, and all matrices in [17] generated randomly, with the entries of $A$, $F \sim \mathcal{N}(0, 1)$ and the entries of $b, u, -\ell \sim \mathcal{U}[0, 1]$, where $\mathcal{U}[0, 1]$ is the uniform distribution over the interval $[0, 1]$, $Q = Q' > 0$, is randomly generated so that its condition number equals $10^3$, and $\mathcal{X} = \{x : \|x_i\|_\infty \leq 3\}$. Algorithm 1 is applied using population-based sampling with $\delta = 0$, $\omega = 0$, $c_i(x) \equiv 1$, $N_i = 10$, $N_{\text{max}} = 30$ for training a feedforward neural network with 3 layers of 10 neurons each and ReLU activation function, without using warm starting while retraining the model. The median RMSE over 50 runs is shown in Figure 3 where it is apparent that IDEAL performs better than the greedy and random methods. Figure 4 shows the polyhedral partition associated with the exact mpQP solution (unknown for active learning) computed as described in [29] along with the queried samples and initial samples generated by one of the runs of Algorithm 1 where it is evident that the acquired points are not distributed uniformly.

4.3 Simple classification problem: Indicator function

In order to test Algorithm 1 on classification problems, we consider data generated by the indicator function $y : \mathbb{R}^2 \to \{0, 1\}$ of the unit circle defined as

$$y(x) = \begin{cases} 1 & \text{if } \|x\|_2^2 \leq 1 \\ 0 & \text{otherwise} \end{cases}$$  \hspace{1cm} (18)$$

Algorithm 1 is applied with $\delta = 5$, $\omega = 0$, $c_i(x) \equiv 1$, $N_i = 10$, $N_{\text{max}} = 100$ to fit a neural network with two layers of ten neurons each and logistic activation and output functions, with warm starting enabled. Pool-based sampling is used on a set $\mathcal{X}_P$ of $M = 1000$ random
Figure 4: mpQP problem \((m = 2)\): exact mpQP solution, queried samples (green circle) and initial samples (red diamonds) feature vectors generated uniformly in \([-2,2] \times [-2,2]\). The median accuracy computed on all vectors \(\bar{x}_i \in \mathcal{X}_P\) over 50 runs is shown in Figure 5 (left plot). Figure 6 (left plot) shows the learned classifier \(\hat{y}\) during one of the tests (cyan curve), the pool \(\mathcal{X}_P\) of samples (gray circles), the queried samples (green dots), and the initial samples (red diamonds). It is apparent that IDEAL spontaneously tends to sample \(\mathcal{X}_P\) on the (unknown) decision boundary of \(y(x)\).

Next, we add an unknown constraint by only defining \(y(x)\) for \(x \in \mathcal{X}\), where

\[
\mathcal{X} \triangleq \{x : 3x_2 \leq \sqrt{3}|x_1|\}
\]  

and repeat the same test, obtaining the median accuracy results shown in Figure 5 (right plot), where accuracy is computed on feasible vectors \(\bar{x}_i \in \mathcal{X}_P \cap \mathcal{X}\). As shown in Figure 6 (right plot), IDEAL spontaneously tends to avoid querying infeasible vectors \(x \in \mathcal{X}_p \setminus \mathcal{X}\).

### 4.4 Real-world datasets

We test the proposed AL approach on real-world datasets from the University of California, Irvine (UCI) Machine Learning Repository for regression and classification summarized in Table 3. For regression problems, we train predictors \(\hat{y}\) with two layers of five neurons.
Figure 5: Classification problem \cite{18}, median accuracy without (left plot) and with unknown constraint \cite{19} (right plot).

| dataset                      | M  | n | m | type |
|------------------------------|----|---|---|------|
| concrete-slump\cite{3}       | 103| 7 | 1 | R    |
| mpg\cite{4}                  | 392| 6 | 1 | R    |
| winequality-white\cite{5}    | 4989| 7 | 1 | R    |
| yacht\cite{6}                | 308| 6 | 1 | R    |
| iris\cite{7}                | 150| 4 | 3 | C    |
| ecoli\cite{8}               | 336| 7 | 8 | C    |
| raisin\cite{9}              | 900| 6 | 1 | C    |
| transfusion\cite{10}        | 748| 4 | 1 | C    |

Table 3: UCI ML datasets: $M =$ number of available samples in the pool, $n =$ number of features, $m = 1$ in the case of regression (R) or the target dimension after one-hot encoding labels in the case of classification (C)

each, for classification predictors $\hat{y}$ with three layers of ten neurons each, with warm starting enabled. In all cases, the logistic activation function and $\ell_2$-regularization term equal to $10^{-2}$ on the vector of weight/bias terms of the model are applied. In all tests, we use pool-based AL with IDEAL parameters $\delta = 5$, $\rho = 0.5$, $N_{init} = 20$, $N_{max} = 100$ (regression tests) or $N_{max} = 60$ (classification tests), and warm start while retraining the predictor. Median results over 50 tests are shown in Figure 7 for regression and in Figure 8 for classification, respectively.

\cite{https://archive.ics.uci.edu/ml/datasets/Concrete+Slump+Test}
\cite{https://archive.ics.uci.edu/ml/datasets/auto+mpg}
\cite{https://archive.ics.uci.edu/ml/datasets/Wine+Quality}
\cite{https://archive.ics.uci.edu/ml/datasets/Yacht+Hydrodynamics}
\cite{https://archive.ics.uci.edu/ml/datasets/Iris}
\cite{https://archive.ics.uci.edu/ml/datasets/Ecoli}
\cite{https://archive.ics.uci.edu/ml/datasets/Raisin+Dataset}
\cite{https://archive.ics.uci.edu/ml/datasets/Blood+Transfusion+Service+Center}
5 Conclusion

In this paper, we have introduced a relatively simple method to solve a very broad set of active learning problems of regression and classification, as it is not linked to any particular class of prediction functions and supports both pool-based and population-based sampling. The objective function driving the optimal selection of the following feature vector only requires evaluating the prediction function that has been currently learned and compare it to the target values acquired so far, an advantage compared to other approaches such as query-by-committee methods in which multiple predictors must be evaluated.

Our practical experience is that for low-dimensional problems (say up to three features) it is usually more efficient to create a large pool of randomly-selected feature vectors and use pool-based active learning, i.e., to optimize the sample acquisition problem by enumeration rather than global optimization. The method also seems to be particularly advantageous to learn functions that have plateaus (such as in classification problems), because the IDW uncertainty terms tend to be small in regions of the feature-vector space where the acquired targets have similar values. While this is an advantage, it also possibly endangers the method, as it may lead to miss areas of significant change in the underlying function. For this reason, as for global optimization using surrogate functions, we found that a safeguard is to weight a pure exploration term ($\delta > 0$), which is entirely independent of the target values acquired and the predictor learned.

Future research will be devoted to adapting the weight on the exploration term automatically while learning, and to extend the method to streaming data, to support online learning problems such as those that arise in recursive identification of dynamical systems.
Figure 7: Regression problems, median RMSE results: concrete-slump (upper left), mpg (upper right), winequality-white (lower left), yacht (lower right)

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Figure 8: Classification problems, median accuracy results: iris (upper left), ecoli (upper right), raisin (lower left), transfusion (lower right)

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