To appear in the proceedings of IJCAI-95

Multiresolution Instance-Based Learning

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Abstract

Instance-based learning methods explicitly remember all the data that they receive. They usually have no training phase, and only at prediction time do they perform computation. Then, they take a query, search the database for similar datapoints and build an on-line local model (such as a local average or local regression) with which to predict an output value. In this paper we review the advantages of instance based methods for autonomous systems, but we also note the ensuing cost: hopelessly slow computation as the database grows large. We present and evaluate a new way of structuring a database and a new algorithm for accessing it that maintains the advantages of instance-based learning. Earlier attempts to combat the cost of instance-based learning have sacrificed the explicit retention of all data, or been applicable only to instance-based predictions based on a small number of near neighbors or have had to re-introduce an explicit training phase in the form of an interpolative data structure. Our approach builds a multiresolution data structure to summarize the database of experiences at all resolutions of interest simultaneously. This permits us to query the database with the same flexibility as a conventional linear search, but at greatly reduced computational cost.

1. Introduction

Instance-based learning methods [Stanfill *et al.*, 1986; Atkeson, 1989; Aha *et al.*, 1991; Moore, 1990] are highly flexible, general purpose techniques for making predictions from earlier data. Instance-based methods (also known as "memory-based" methods or "lazy-learning" methods, and closely related to "case-based" methods) explicitly remember all the data they are shown. Only at prediction time do they perform non-trivial amounts of computation. This behavior differs from more conventional machine learning algorithms, in which training occurs between the reception of data and prediction. Examples of instance-based methods are nearest neighbor, kernel regression, and locally weighted linear regression. Example of non-instance-based techniques (they have a training phase) are neural networks and decision trees. Instance based methods can sometimes be a preferable form of function approximator. There are three main reasons for this:

Flexible Inductive Bias
With very little data, a method such as nearest neighbor gives sensible, conservative predictions: it does not wildly extrapolate. But as the amount of data increases, so does the complexity of the function that nearest neighbor can approximate. This contrasts with, for example, multi-layer neural networks that do not by default have this property of representative power increasing locally according to the amount of local data. In the limit, very local methods can learn any piecewise continuous function to arbitrary precision (although with high dimensional, uniformly distributed input the amount of data to do this can be enormous). For practical use in function approximation, much better instance-based methods than nearest neighbor are available that form local linear models, and compute weighted averages of data to remove the noise from predictions (e.g, see [Atkeson, 1989; Grosse, 1989]).

Learning parameters need not be fixed in advance
There are many learning parameters in instance-based algorithms. One of the most important concerns the extent to which the smoothing of noise is traded against goodness of fit. Others include (i) the parameters of a distance metric for determining the similarity between an input point and the query and (ii) the discrete decision of which attributes are relevant. Instance-based methods do not need to decide on these learning parameters in advance. They can use whichever parameters they desire for one prediction and then have the option of using an entirely different set for another prediction. This is of immense use in an autonomous system that is both making new predictions online and tuning its learning parameters online as new data is arriving [Moore *et al.*, 1992]. In contrast, a non-instance-based method must choose a parameter set and then train with it. If a different parameter set is later needed then it is necessary for a non-instance-based method to retrain itself (and it is therefore also necessary for it to remember all previous data).

Instance-based can cover the global-local spectrum
Instance-based methods do not necessarily have to be local predictors, based on a small handful of local datapoints. This is particularly important for large numbers of attributes, highly noisy data, and for small databases. Many of our own applications involve very noisy systems in which the underlying function is non-linear but generally smooth. In these cases the best instance-based function approximator might, for example, use the closest 30% of all datapoints to the query to form its prediction. In

some extreme cases, for example if the underlying function were nearly linear and local linear regression was in use, this figure might increase to 80% of the datapoints---essentially a global, not local, function approximator.

The properties described above make instance-based methods particularly desirable for autonomous systems that spend their lives in environments that are not known in advance and in which the designers will not be able to manually tweak the learning parameters during operation.

Unfortunately, instance-based methods have a serious problem. As the database grows large it becomes increasingly expensive to make predictions. Each prediction involves searching the database to find similar earlier datapoints. This can mean hopelessly slow performance after merely tens of thousands of predictions. Various researchers have attempted to deal with this problem [Aha *et al*., 1991; Grosse, 1989; Moore, 1990; Skalak, 1994], but, as we will see in Section 7, none in a manner that avoids sacrificing at least one of the benefits of instance-based methods described above. This paper describes a new solution, based on a multiresolution hierarchical structuring of data, which retains all the above properties of instance-based learning while providing fast instance-based performance. Asymptotically it reduces the cost of a query from linear to logarithmic in the number of datapoints.

2. Kernel Regression

The approach taken in this paper can be applied to a wide variety of instance-based algorithms, but here we will concentrate on one of the most well known examples: Kernel Regression (see, for example, [Franke, 1982]). Assume that datapoints consist of {input, output} pairs such as $(\mathbf{x}_1,y_1)$, $(\mathbf{x}_2,y_2)$,. . . $(\mathbf{x}_N,y_N)$ where the inputs are *d*-element real-valued vectors and the outputs are scalars, and to date we have observed *N* datapoints. The prediction problem is: given an input vector $\mathbf{x}_q$, which is called the *query*, how to predict the output $y^{est}(\mathbf{x}_q)$?

The *k*-nearest neighbor solution to this problem would be to find the *k* datapoints that have input vectors closest to the query and to take the average of the corresponding output values as $y^{est}(\mathbf{x}_q)$. Kernel regression uses a similar idea except that a *weighted average* of all the points in the database is used, and the points closest to the query are assigned the largest weight. Thus:

$$y^{\text{est}}(x_q) = \frac{\sum w_i y_i}{\sum w_i}$$

where w_i is the weight assigned to the *i*th datapoint in our memory, and is large for points close to the query and almost zero for points far from the query. It is calculated as a decreasing function of Euclidean distance, for example by a gaussian:

$$w_i = \exp\left(-\frac{\text{Distance}^2(x_q, x_i)}{2K^2}\right)$$

The bigger the parameter *K* is, the flatter the weight function curve is, which means that many memory points contribute quite evenly to the regression. As *K* tends to infinity the predictions approach the global average of all points in the database. If the *K* is very small, only closely neighboring datapoints make a significant contribution.

K is an important smoothing parameter for kernel regression. If the data is relatively noisy, we expect to obtain smaller prediction errors with a relatively large *K*. If the data is noise free then a small *K* will avoid smearing away fine details in the function. This is illustrated in Figure 1.

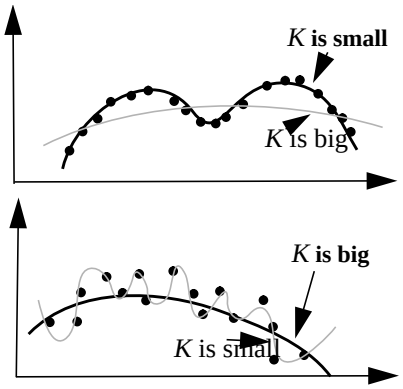


Figure 1: For the noiseless data in the top example, a small K gives the best regression (in terms of future predictive accuracy). For the noisy data in the bottom example, a larger K is preferable.

The drawback of kernel regression is the expense of enumerating all the distances and weights from the memory points to the query. Several methods have been proposed to address this problem, reviewed in Section 7.

3. Multiresolution structuring of datapoints

The main idea of multiresolution instance-based regression is grouping. The following figure shows a 2-d input space case. Given a query, based on the distance from each point to the query, we could calculate a weight for every point in the input space.

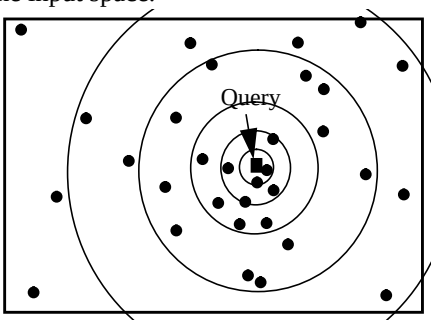


Figure 2: Grouping data according to distance from query.

If we split space into several rings as illustrated, we will see that for each group or ring, all the individual weights inside are approximately equal. Assume we have a group with *n* datapoints in which we know that all weights in the group are close to the same value *w*. Let the *i*th member of the group have weight $w_i = w + \varepsilon_i$ where all ε_is are small. When performing kernel regression we need to accumulate two sums over all datapoints in the database:

$$\sum w_i y_i \qquad \text{and} \qquad \sum w_i$$

The former of these sums will then be divided by the latter. Let us consider how we can compute the contribution to these sums from all the points in our current group. Restricting our attention to summations over the *n* points in the current group we have

$$\sum w_i y_i = \sum \left(\bar{w} + \varepsilon_i \right) y_i = \bar{w} \sum y_i + \sum \varepsilon_i y_i \quad \text{and}$$

$$\sum w_i = \sum \left(\bar{w} + \varepsilon_i \right) = n\bar{w} + \sum \varepsilon_i$$

Providing we know *n*, *w* and Σy_i for the current group we can therefore compute an approximation to $\Sigma w_i y_i$ and Σw_i in constant time without needing to sum individual members of the group. This approximation to the partial sums is good to the extent that $\Sigma \varepsilon_i y_i$ is small with respect to $w\Sigma y_i$ and $\Sigma \varepsilon_i$ is small with respect to *nw*.

Kd-trees for grouping

We now understand that if we are given a query, and if someone has structured the set of datapoints into groups for which, relative to the current query, all weights in each group are very similar, then we can compute approximations to the sums $\sum w_i y_i$ and $\sum w_i$ in time proportional to the number of groups instead of the number of individual datapoints. But how can such a set of groupings be obtained? And how can we ensure that all weights within each grouping are very similar?

We can use a *k*d-tree [Preparata *et al*., 1985], enhanced with extra cached information, as an implementation of this grouping idea. A *k*d-tree is a binary tree that recursively splits the whole input space into partitions, in a manner similar to a decision tree acting on real-valued inputs. Each node in the *k*d-tree represents a certain partition of the input space; the children of this node denote subsets of the partition. Hence, the root of the *k*d-tree is the whole input space, while the leaves are the smallest possible partitions this *k*d-tree offers. The tree is built in a manner that adapts to the local density of input points and so the sizes of partitions at the same level are not necessarily equal to each other.

Instead of dividing the input space into rings, we use hyper-rectangles within the *k*d-tree to implement the grouping idea. The groups are internal nodes of the *k*d-tree. Which nodes are selected for a given query? They are chosen to be nodes that represent hyper-rectangles in input space over which the weight function (relative to the current query) varies little. Hence, at parts of state space with a highly varying weight function (often the part near the query) we use leaves or lower-level internal nodes---small-sized partitions. And at parts of state space with little variation in the weight function (often the parts far from the query) we use the higher-level internal nodes. This is illustrated in figure 3.

When the query, *Q*, is at the top-right corner of the input space in our diagram, the circled nodes in the tree are the groups used for the prediction. The radii of the circles depend on the distances from the hyper-rectangles to the query. For a different query, *Q**, we use different groupings, shown by nodes with a * mark.

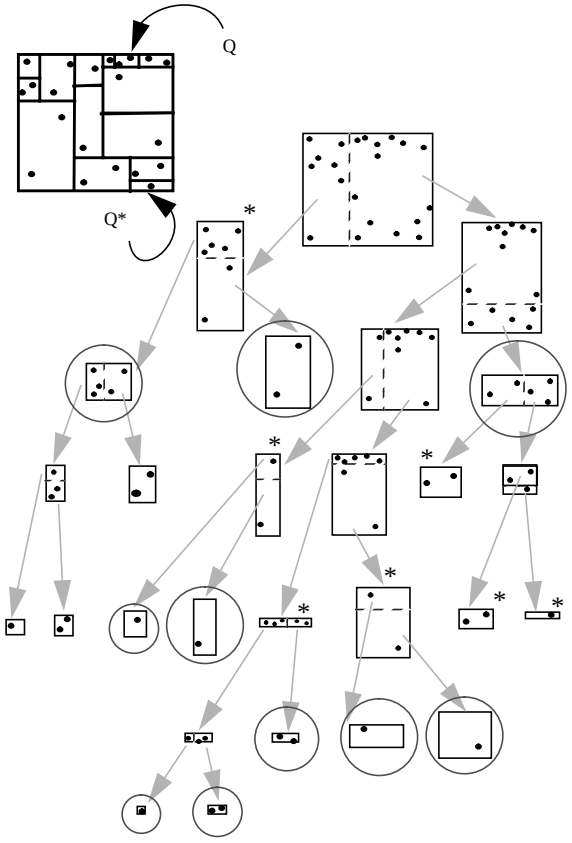


Figure 3. To implement the grouping idea, we use hyper-rectangles with *k*d-tree. Lower-level nodes or leaves are chosen (circled) to present the partition of input space closer to the query. For different query (with *), we can use the same kd-tree but choose different nodes.

Kernel Regression Trees Defined

Each node of the *k*d-tree denotes a hyper-rectangle of input space, and also is defined to contain all datapoints that have input vectors inside this hyper-rectangle. The root node covers the whole of input space and contains all the datapoints. The leaf nodes explicitly record the datapoints

that reside in the leaf.

Each node records the hyper-rectangle covered by it. This is defined as the smallest bounding box that contains all the datapoints owned by this node of the tree.

Each non-leaf node has two children representing two disjoint subregions of the parent node. The break between the children is defined by two values. **`split_d`** is the splitting dimension, and determines which component of input space (which "attribute") the children will be split upon. **`split_v`** determines the numerical value at which each split occurs, The datapoints owned by the left child of a node are those datapoints owned by the node which are less than value **`split_v`** in input component **`split_d`**. The right child contains the other datapoints.

Finally, each node contains two other pieces of information: **`n_below`**, the number of datapoints below the current node, and **`sum`**, the sum Σy_i of all output values of datapoints contained in this node. These are two of the three values needed to compute the contribution of a group to the partial sums in kernel regression. The third component, *w,* depends upon the location of the query and is determined dynamically in a manner described shortly.

Constructing the kernel regression tree

To construct a tree from a batch of training instances we use a top-down recursive procedure. This is the most standard way of constructing *k*d-trees, described, for example, in [Preparata *et al*., 1985; Omohundro, 1991]. In this work we use the common variation of splitting a hypercube in the center of the widest dimension instead of at the median point. This method of splitting does not guarantee a balanced tree, but leads to generally more cubic hyper-rectangles, which has empirically proved better than other schemes (pathological imbalances are conceivable, but trivial modifications to the algorithm prevent that). The cost of making a tree from *N* datapoints is *O(N log N)*.

The base case of the recursion occurs when a node is created with $N_{\min}$ or fewer datapoints. Then those datapoints are explicitly stored in the leaf node. In our experiments $N_{\min} = 2$.

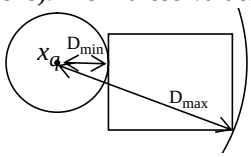
To incrementally add a new datapoint to the tree, the leaf node containing the point is determined (*O(log N)* cost). The datapoint is inserted there (and a new subtree is recursively built if the number of nodes exceeds $N_{\min}$). Then all ancestors of the updated node are updated to maintain consistency in their hyper-rectangles, **`sum`** and **`n_below`** values.

4. Computing the kernel regression sums

Given a query point $\mathbf{x}_q$ we are required to compute Σw_i and $\Sigma w_i y_i$, summed over all datapoints in the tree and then divide the latter by the former. This is performed by a top-down search over the tree. At each node we make a decision between:

1. (Cutoff) Treat all the points in this node as one group (a cheap operation) or
2. (Recurse) search the children.

We will use the cutoff option if we are confident that all weights inside the node are similar. Given the current query $\mathbf{x}_q$ and the hyper-rectangle of the current node it is an easy matter to compute $D_{\min}$ and $D_{\max}$: the minimum and maximum possible distances of any datapoint in this node to the query (computational cost is linear in the number of dimensions). From these values one can then compute the minimum and maximum possible weights $w_{\min}$ and $w_{\max}$ of any datapoints owned by this node, since the weight of a point is a decreasing function of distance to the query. We thus decide if $w_{\min}$ and $w_{\max}$ are close enough to warrant the cut-off option.



The search is thus a recursive procedure which returns two values: *sum-weights* and *sum-wy.* If the cutoff option is taken, then estimate the weight of all datapoints as $\bar{w} = (w_{min} + w_{max})/2$ and return:

$$\textit{sum-weights} = \texttt{n\_below} \times \bar{w}$$

$$\textit{sum-wy} = \texttt{sum} \times \bar{w}$$

If the cutoff option is not taken, recursively compute *sum-weights* and *sum-wy* for the left and right children, and then return:

$$\textit{sum-weights} = \textit{sum-weights(left)} + \textit{sum-weights(right)}$$

$$\textit{sum-wy} = \textit{sum-wy(left)} + \textit{sum-wy(right)}$$

5. Search Cutoffs

Section 3 described how we can make our approximation arbitrarily accurate by bounding the maximum deviation we will permit from the true weight estimate with a value $\varepsilon_{\max} > 0$ and then making $\varepsilon_{\max}$ arbitrarily small. Thus the simplest cutoff rule in the *k*d-tree search would be to cutoff if $w_{\max} - w_{\min} < \varepsilon_{\max}$. It is easy to show that this guarantees that the total sum of absolute deviations $|\Sigma\varepsilon_i|$ is less than $N_T\varepsilon_{\max} / 2$ where N_T is the number of points in the tree. There are, however, other possible cutoff criteria which provide arbitrary accuracy in the limit, but which, when used as an approximation, have more satisfactory properties.

The simple cutoff rule does not take into account that a larger total error will occur if the node contains very many points than if the node contains only a few points. It does also not account for the fact that in a practical case we are less concerned about the absolute value of the sum of deviations $|\Sigma\varepsilon_i|$ but rather the size of $|\Sigma\varepsilon_i|$ relative to the sum of the weights Σw_i. Some simple analysis reveals a cutoff cri-

terion to satisfy both of these intuitions. Cutoff only if

$$(w_{\max} - w_{\min})\, N_B < \tau\, \Sigma w_i$$

where N_B is the number of datapoints below the current node. Simple algebra reveals that this guarantees

$$|\, \Sigma \varepsilon_i \,| < 0.5\, G\, \tau\, \Sigma w_i$$

where G is the number of groups finally used in the search (and thus $G < N_T$, hopefully considerably less). Notice that this cutoff rule requires us to know Σw_i in advance, which of course we do not. Fortunately the sum of weights obtained so far in the search can be used as a valid lower bound, and so the real algorithm makes a cutoff if:

$$\frac{(w_{\max} - w_{\min})\, N_B}{\text{weight so far in search}} < \tau$$

where τ is a system constant.

6. Experiments and results

Let us review the performance of the multiresolution method in comparison to kernel regression. In the first experiment we use a trigonometric function of two inputs with added noise: $\boldsymbol{x}_i$ = uniformly generated random vector with all components between 0 and 100 and y_i = a function of $\boldsymbol{x}_i$ (which ranges between 0 and 100 in height), with gaussian noise of standard deviation 10.

10,000 datapoints were generated. Experiments were run for different values of kernel width *K*. In all experiments, the cutoff threshold τ was 0.005. Figure 4a shows the test-set error on 1000 test points for both regular kernel regression ("Regular KR") and multiresolution kernel regression ("Multires KR") graphed for different values of *K*. The values are very close, indicating that multires KR is providing, for a wide range of kernel widths, a very close approximation to regular KR. Figure 4b shows the computational cost (in terms of the summations that dominate the cost of KR) of the two methods. Regular KR sums all points, and so is a constant 10,000 in cost. Multires KR is substantially cheaper for all values of *K*, but particularly so for very small and very large values.

Figures 5a and 5b show corresponding figures for a similar trigonometric function of five inputs. This still shows similar prediction performance as regular KR. The cost is still always less than regular KR, but in the worst case the computational saving is only a factor of three (when $K = 40$, multires KR cost = 3,200). This is not an especially impressive result. However, for any fixed dimensionality and kernel width, costs rise sub-linearly (in principle logarithmically) with the number of datapoints. To check this, we ran the same set of experiments for a dataset of ten times the size: 100,000 points. The results, in Figure 6, show that with this large increase in data, the effectiveness

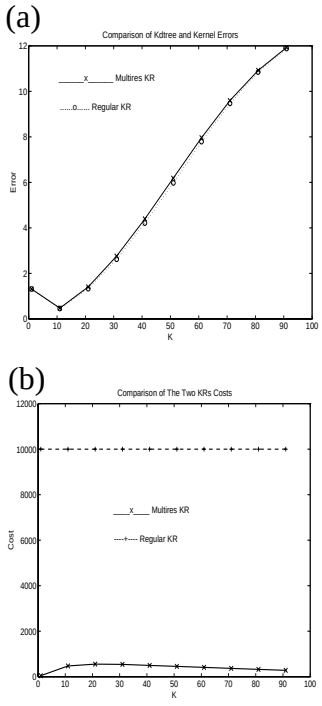


Figure 4.. Comparison between (a) error and (b) cost of regular KR versus multires KR for 2-d inputs, for a dataset of size 10,000.

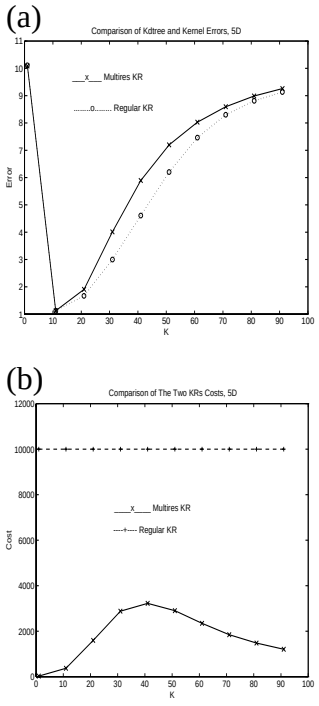


Figure 5: Comparison between error and cost of regular KR versus multires KR for 5-d inputs, for a dataset of size 10,000.

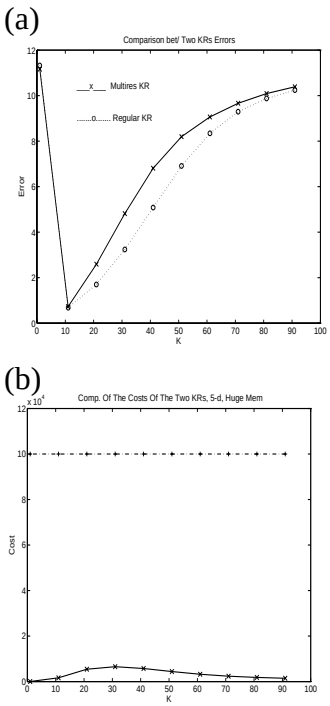


Figure 6: The same experiment as Figure 5, except with ten times the amount of data: 100,000 datapoints

of multires KR becomes more apparent. For example, consider the K = 40 case. With 100,000 datapoints instead of 10,000, the cost is only increased from 3,200 to 5,700 while the cost of regular KR (of course) increased from 10,000 to 100,000.

Investigating the t threshold parameter

Next, we will examine the effect of the τ parameter on the behavior of the algorithm. As τ is increased we expect the computational cost to be reduced, but at the expense of the accuracy of the predictions in comparison to the regular KR. The results in Figure 7 agree with this expectation: the left hand graph shows that for 2-d, 3-d, 4-d and 5-d datasets (each with 10,000 points) the proportional error between multires and regular regression increases with τ. The right hand graph shows a corresponding decrease in computational cost.

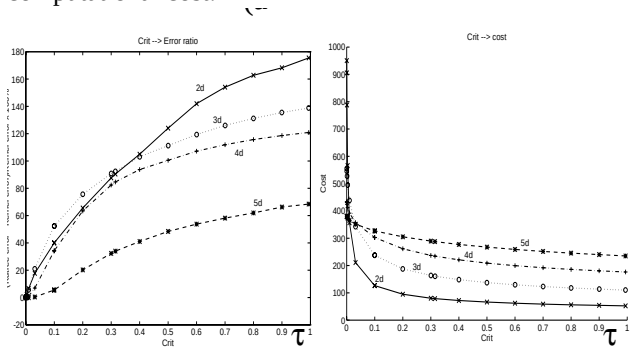


Figure 7. (Upper) the relative accuracy and (lower) the computational cost of multires KR against τ--the cutoff threshold.

Real datasets

In another experiment, we ran multires KR on data from several real-world and robot-learning datasets. Further details of the datasets can be found in [Maron and Moore, 1994]. They include an industrial packaging process for which the slowness of prediction had been a reasonable cause for concern. Encouragingly, multires KR speeds up prediction by a factor of 100 with no discernible difference in prediction quality between multires and regular KR. This and other results are tabulated below. The costs and RMS values given are averages taken over an independent test set. Notably, the datasets with the least savings were **pool**, which had few datapoints, and **robot**, which was high dimensional.

Domain	Number Points	Dimension	KR Cost	MRes Cost	KR rms err	MRes rms err
Energy	2144	5-d	2144	232.9	1.687	1.690
Package	32000	3-d	32000	289.0	6.07	6.09
Pool	213	3-d	213	50.7	2.125	2.123
Protein	4664	3-d	4664	383.8	1.036	1.106
Robot	871	14-d	871	225	6.354	6.976

High dimensional, non-uniform data

Our final experiment concerned the question of how well the method performs if the number of input variables is relatively large, but if the attributes are not independent. For example, a common scenario in robot learning is for the input vectors to be embedded on a lower-dimensional manifold. We performed two experiments, each with 9 inputs and 10,000 datapoints. In the first experiment, the components of the input vectors were distributed uniformly randomly. In the second experiment the input vectors were distributed on a non-linear 2-d manifold of the 9-d input space. The results were:

	9-d uniform	9-d inputs on 2d manifold
Regular KR cost	10,000	10,000
Multires KR cost	3,100	430
Regular KR mean testset error	13.07	1.06
Multires KR mean testset error	13.08	1.15

The results indicate that, as would be expected, the cost advantage of multires KR is not large (a factor of 3) for 9-d uniform inputs, but is far better if the inputs are distributed within a lower-dimensional space.

7. Related Work and Discussion

There has not been room in this paper to discuss a number of additional flexibilities that multires KR provides. Once the *k*d-tree structure is built, it is possible to make different queries with not only different kernel widths *K*, but also different Euclidean distance metrics, with subsets of attributes ignored, or with some other distance metrics such as Manhattan. It is also possible to apply the same technique with different weight functions and for classification instead of regression.

It should be remembered that although we have succeeded in reducing the cost of instance-based learning, there are other methods (outlined below) in the literature for doing so. Why might Multires be preferable? This depends upon the extent to which the application needs the following advantages of instance based learning described in Section 1:

- Flexibility to work throughout the local/global spectrum.
- The ability to make predictions with different parameters without needing a retraining phase.

Multires provides for both. No other software method, to our knowledge, does. There is, however, the simple hardware alternative of using a fast enough computer. The standard kernel regression method can be parallelized with full efficiency.

*K*d-trees have frequently been used in instance-based learning methods for nearest neighbor searching or for range searching [Preparata *et al*., 1985]. The range-search solution to kernel regression is to find all points in the *k*d-tree that have a significant weight, and then only sum

together the weighted components of those points. This is only practical if the kernel width K is small. If it is large, all the datapoints may have a significant weight, but only a small local variation in weight. Range searching would sum all the points individually. Multires would visit only relatively large intermediate nodes (because the weight variation is locally low) and so would still be cheap. Even in cases of small kernel widths and large amounts of data the multiresolution method can be preferable to the range search method because it may not need to search all the way down to the leaf nodes.

Another solution to the cost of instance-based learning is *editing* (or *prototypes*): most datapoints are forgotten and only particularly representative ones are used (e.g. [Kibler and Aha, 1988; Skalak, 1994]). Kibler and Aha extended this idea further by allowing datapoints to represent local averages of sets of previously-observed datapoints. This can be effective, and unlike range-searching can be applicable even for wide kernel widths. However, the degree of local averaging must be decided in advance: unlike Multires, queries cannot occur with different kernel widths without rebuilding the prototypes. A second occasional problem is that if we require very local predictions, the prototypes must either lose local detail by averaging, or else all the datapoints are stored as prototypes.

There are interesting parallels between prototypes and Multires. The intermediate nodes of the *k*d-tree can be thought of as fabricated prototypes, summarizing all the data below them.

Decision trees and *k*d-trees have been previously used to cache local mappings in the tree leaves [Grosse, 1989; Moore, 1990; Omohundro, 1991; Quinlan, 1993]. These algorithms provide fast access once the tree is built, but a new structure needs to be built each time new learning parameters are required. Furthermore, unlike the multiresolution method, the resulting predictions from the tree have substantial discontinuities between boundaries. Only in [Grosse, 1989] is continuity enforced, but at the cost of tree-size, tree-building-cost and prediction-cost all being exponential in the number of input variables.

Dimensionality is a weakness of Multires. Diminishing returns set in above approximately 10 dimensions if the data is distributed uniformly. This is an inherent problem for which no solution seems likely because uniform data in high dimensions will have almost all datapoints almost exactly the same distance apart, and a useful notion of locality breaks down.

This paper discussed an efficient implementation of kernel regression. We are applying exactly the same algorithm to locally weighted polynomial regression, in which a prediction fits a local polynomial to minimize the locally weighted sum squared error. The only difference is that each node of the *k*d-tree stores the regression design matrices of all points below it in the tree. This permits fast prediction and also fast computation of confidence intervals and analysis of variance information.

Multires as described here is only applicable to numeric features. An interesting avenue for future work would be ways to extend the method to binary or symbolic features.

8. Conclusion

Instance based methods make use of a database of multidimensional data. Multiresolution instance-based methods provide a means for performing queries quickly, even when the amount of data is enormous. An important message of this paper is that for efficient accessing of large instance bases (or case bases, or memory-bases) it is not necessary to resort to throwing data away. Intelligent structuring is an alternative.

Acknowledgement

We wish to thank the IJCAI reviewers for insightful and useful comments. This work was support by a research gift from 3M corporation and an NSF Reserach Initiation Award.

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