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Data Mining using $\mathcal{MLC}$++ A Machine Learning Library in C++

`http://www.sgi.com/Technology/mlc`

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Abstract

Data mining algorithms including machine learning, statistical analysis, and pattern recognition techniques can greatly improve our understanding of data warehouses that are now becoming more widespread. In this paper, we focus on classification algorithms and review the need for multiple classification algorithms. We describe a system called $\mathcal{MLC}$++, which was designed to help choose the appropriate classification algorithm for a given dataset by making it easy to compare the utility of different algorithms on a specific dataset of interest. $\mathcal{MLC}$++ not only provides a workbench for such comparisons, but also provides a library of C++ classes to aid in the development of new algorithms, especially hybrid algorithms and multi-strategy algorithms. Such algorithms are generally hard to code from scratch. We discuss design issues, interfaces to other programs, and visualization of the resulting classifiers.

Keywords: data mining, machine learning, classification, benchmark.

1 Introduction

Data warehouses containing massive amounts of data have been built in the last decade. Many organizations, however, find themselves unable to understand, interpret, and extrapolate the data to achieve a competitive advantage. Machine learning methods, statistical methods, and pattern recognition methods provide algorithms for mining such databases in order to help analyze the information, find patterns, and improve prediction accuracy.

One problem that users and analysts face when trying to uncover patterns, build predictors, or cluster data is that there are many algorithms available and it is very hard to determine which one to use. We detail a system called $\mathcal{MLC}$++, a Machine Learning library in C++ that was designed to aid both algorithm selection and development of new algorithms.

The $\mathcal{MLC}$++ project started at Stanford University in the summer of 1993 and is currently public domain software (including sources). A brief description of the library and plan was given in Kohavi, John, Long, Manley & Pfleger (1994). The distribution moved to Silicon Graphics in late 1995. Dozens of people have used it, and over 300 people are on the mailing list.

We begin the paper with the motivation for the $\mathcal{MLC}$++ library, namely the fact that there cannot be a single best learning algorithm for all tasks. This has been proven theoretically and shown experimentally. Our recommendation to users is to actually run the different algorithms. Developers can use $\mathcal{MLC}$++ to create new algorithms suitable for their specific tasks.

In the second part of the paper we describe the $\mathcal{MLC}$++ system and its dual role as a system for end-users and algorithm developers. We show a large comparison of 22 algorithms on eight large datasets for the UC Irvine repository (C. Blake & Merz 1998). A study of this magnitude would be extremely hard to conduct without such a tool, yet with $\mathcal{MLC}$++, it was mostly a matter of CPU cycles and a few scripts to parse the output. Our study shows the behavior of different algorithms on different datasets and stresses the fact that while there are no clear winners, some algorithms are (in practice) better than others on these datasets. More importantly, for each *specific* task, it is relatively easy to choose the best algorithms to use based on accuracy estimation and other utility measures (*e.g.*, comprehensibility).

In the third part of the paper we discuss the software development process in hindsight. We were forced to make many choices on the way and briefly describe how the library evolved. We conclude with related work.

2 The Best Algorithm for the Task

In theory, there is no difference between theory and practice; In practice, there is
—Chuck Reid

Statements that one classifier structure is better than another, such as "rules are much more than decision trees" made by Parsaye (1996) are usually irrelevant and often misinterpreted. There are two problems with such claims: what is "better" and how the semantics of "better" relate to learning:

What is better Several criteria can be used for comparing structures, such as comprehensibility and compactness. For some applications, such as medical domains, it is probably important to understand the classifiers whereas for others, such as hand writing recognition, it is not very important. Compactness may or may not be important. Two chained neurons may compactly represent a target that would be hard to understand by many people. Rules are known to be more compact than decision trees when one is looking at the leaves as rules described by the path from the root. However, a decision tree provides a natural structure and data segmentation that can help users group rules together and look at them hierarchically.

Relevance to learning The fact that one structure is more general or more powerful does not imply that it is easier to learn; in fact, the opposite is true: more powerful structures are provably harder to learn in some frameworks, such as Valiant's Probably Approximately Correct framework (Valiant 1984, Kearns & Vazirani 1994). Inductive Logic Programming models (Lavrac & Dzeroski 1994, Muggleton 1992) are more powerful than propositional learning methods, yet very few practical systems are available that are as accurate as propositional systems. Most learning algorithms attempt to solve NP-hard problems (Garey & Johnson 1979) using heuristics such as limited lookahead. It is still unclear how general the heuristics are and when they will lead to solutions that are far from the global optimum.

Theoretical results show that there is not a single algorithm that can be uniformly more accurate than others in all domains. Although such theorems are of limited applicability in practice, very little is known about which algorithms to choose for specific problems.

We claim that unless an organization has specific background knowledge that can help it choose an algorithm or tailor an algorithm based on specific needs, it should simply try a few of them and pick the best one for the task.

2.1 There is Not a Single Best Algorithm Overall

There is a theoretical result that no single learning algorithm can outperform any other when the performance measure is the expected generalization accuracy. This result, sometimes called the No Free Lunch Theorem or Conservation Law (Wolpert 1994, Schaffer 1994), assumes that all possible targets are equally likely. A brief review of theoretical results is presented in Appendix A.

In practice, of course, the user of a data mining tool is interested in accuracy, efficiency, and comprehensibility for a specific domain, just as the car buyer is interested in power, gas mileage, and safety for specific driving conditions. Averaging an algorithm's performance over all target concepts, assuming they are all equally likely, would be like averaging a car's performance over all possible terrain types, assuming they are all equally likely. This assumption is clearly wrong in practice; for a given domain, it is clear that not all concepts are equally probable.

In medical domains, many measurements (attributes) that doctors have developed over the years tend to be independent: if the attributes are highly correlated, only one attribute will be chosen. In such domains, a certain class of learning algorithms might outperform others. For example, Naive-Bayes seems to be a good performer in medical domains (Kononenko 1993). Quinlan (1994) identifies families of *parallel* and *sequential* domains and claims that neural-networks are likely to perform well in parallel domains, while decision-tree algorithms are likely to perform well in sequential domains.

Therefore, although a single induction algorithm cannot build the most accurate classifiers in all situations, some algorithms will be clear winners in specific domains, just as some cars are clear winners for specific driving conditions. One is usually given the option to test-drive a range of cars because it is not obvious which car will be best for which purpose. The same is true for data mining algorithms. The ability to easily test-drive different algorithms was one of the factors that motivated the development of $\mathcal{MLC}$++.

2.2 Take Each Algorithm for a Test Drive

First, decide on the type of vehicle—a large luxury car or a small economy model, a practical family sedan or a sporty coupe... at this point you're ready for your first trip to a dealership—but only for a test drive...
—Consumer Reports 1996 Buying Guide: How to Buy a New Car

Organizations mine their databases for different reasons. We note a few that are relevant for classification algorithms:

Classification accuracy The accuracy of predictions made about an instance. For example, whether a customer will be able to pay a loan or whether he or she will respond to a yet another credit card offer. Using methods such as holdout, bootstrap, and cross-validation (Weiss & Kulikowski 1991, Efron & Tibshirani 1995, Kohavi 1995*b*), one can estimate the future prediction accuracy on unseen data quite well in practice.

Comprehensibility The ability for humans to understand the data and the classification rules induced by the learning algorithm. Some classifiers, such as decision rules and decision trees are inherently easier to understand than neural networks. In some domains (*e.g.*, medical), the black box approach offered by neural networks is inappropriate. In others, such as handwriting recognition, it is not as important to understand why a prediction was made so long as it is accurate.

Compactness While related to comprehensibility, one does not necessarily imply the other. A Perceptron (single neuron) might be a compact classifier, yet given an instance, it may be hard to understand the labelling process. Alternatively, a decision table (Kohavi 1995*a*) may be very large, yet labelling each instance is trivial: one simply looks it up in the table.

Training and classification time The time it takes to classify versus the training time. Some classifiers, such as neural networks are fast to classify but slow to train. Other classifiers, such as nearest-neighbor algorithms and other *lazy* algorithms (see Aha (1997) for details), are usually fast to train but slow in classification.

Given these factors, one can define a utility function to rank different algorithms (Fayyad, Piatetsky-Shapiro & Smyth 1996). The last step is to test drive the algorithms and note their utility for *your specific domain problem.* We believe that although there are many rules of thumb for choosing algorithms, choosing a classifier should be done by testing the different algorithms, just as it is best to test-drive a car. $\mathcal{MLC}$++ is analogous to your friendly car dealer, only more honest.

3 $\mathcal{MLC}$++ for End-Users

The computer industry has not noticed the deteriorating quality of their products, partly due to the frog factor: Drop a frog in boiling water and it will jump out instantly. Put it in tepid water and raise the temperature slowly, and the frog will sit there staring at you while you boil it to death. With quality ebbing away slowly, we failed to notice the heat
—Tognazzini (1994)

While $\mathcal{MLC}$++ is useful for writing new algorithms, most users simply use it to test different learning algorithms. Pressure from reviewers to compare new algorithms with others led us to interface *external inducers,* which are induction algorithms written by other people. $\mathcal{MLC}$++ provides the appropriate data transformations and the same interface to these external inducers. Thus while you will not find every type of car in our dealership, we provide shuttle service to take you to many other dealerships so you can easily test their cars.

3.1 Inducers

The following induction algorithms were implemented in $\mathcal{MLC}$++:

Const A constant predictor based on majority.

Decision Table A simple lookup table. A simple algorithm that is useful with feature subset selection.

ID3 The decision tree algorithm based on Quinlan (1986). It does not do any pruning.

Lazy decision trees An algorithm for building the "best" decision tree for every test instance described in Friedman, Kohavi & Yun (1996).

Nearest-neighbor The classical nearest-neighbor with options for weight setting, normalizations, and editing (Dasarathy 1990, Aha 1992, Wettschereck 1994).

Naive-Bayes A simple induction algorithm that assumes a conditional independence model of attributes given the label (Domingos & Pazzani 1997, Langley, Iba & Thompson 1992, Duda & Hart 1973, Good 1965).

1R The 1R algorithm described by Holte (1993).

OODG Oblivous read-Once Decision Graph induction algorithm described in Kohavi (1995*c*).

Option Decision Trees The trees have *option* nodes that allow several optional splits, which are then voted as experts during classification (Kohavi & Kunz 1997).

Perceptron The simple Perceptron algorithm described in Hertz, Krogh & Palmer (1991).

Winnow The multiplicative algorithm described in Littlestone (1988).

The following external inducers are interfaced by $\mathcal{MLC}$++:

C4.5 The C4.5 decision-tree induction by Quinlan (1993).

C4.5-rules The trees to rules induction algorithm by Quinlan (1993).

CART The commercial version of CART (Breiman, Friedman, Olshen & Stone 1984) from Salford system was interfaced. In the experiments we have used version 2.0 with a memory limit of 50,000,000 4-word workarea (200MB). The CVLEARN parameter was increased to be larger than the training set size so that the more accurate cross-validation estimation would be used for the pruning phase.

CN2 The direct rule induction algorithm by Clark & Niblett (1989) and Clark & Boswell (1991).

IB The set of Instance Based learning algorithms (Nearest-neighbors) by Aha (1992).

Neural network: Aspirin Migraines The Aspirin/MIGRAINES neural network environment version 6.0 from 29 Aug 1996 uses standard backpropagation (Hertz et al. 1991, Rumelhart, Hinton & Williams 1986). The interface is very simple: the nominal attributes are converted to local encoding and the network constructed contains three layers with the hidden layer containing k nodes. k is automatically set to the number of input and output nodes divided by two, which is a commonly mentioned rule of thumb. Although this rule of thumb is often criticized (*e.g.*, `ftp://ftp.sas.com/pub/neural/FAQ.html`), there are no other good candidates for automatically selecting this number and for comparison purposes we wanted to avoid manual tuning.

OC1 The Oblique decision-tree algorithm by Murthy, Kasif & Salzberg (1994).

PEBLS Parallel Exemplar-Based Learning System by Cost & Salzberg (1993).

Ripper Ripper is a rule-learning system by Cohen (1995).

T2 The two-level error-minimizing decision tree by Auer, Holte & Maass (1995).

Not all algorithms are appropriate for all tasks. For example, Perceptron and Winnow are limited to two-class problems, which reduces their usefulness in many problems we encounter, including those tested in Section 3.5.

3.2 Wrappers and Hybrid Algorithms

Because algorithms are encapsulated as C++ objects in $\mathcal{MLC}$++, we were able to build useful wrappers. A *wrapper* is an algorithm that treats another algorithm as a black box and acts on its output. Once an algorithm is written in $\mathcal{MLC}$++, a wrapper may be applied to it with no extra work.

The two most important wrappers in $\mathcal{MLC}$++ are accuracy estimators and feature selectors. Accuracy estimators use any of a range of methods, such as holdout, cross-validation, or bootstrap to estimate the performance of an inducer (Kohavi 1995*b*). Feature selection methods run a search using the inducer itself to determine which attributes in the database are useful for learning. The wrapper approach to feature selection automatically tailors the selection to the inducer being run (John, Kohavi & Pfleger 1994, Kohavi & John 1997).

A voting wrapper runs an algorithm on different portions of the dataset and lets them vote on the predicted class (Wolpert 1992, Breiman 1996*b*, Perrone 1993, Ali 1996). A discretization wrapper pre-discretizes the data, allowing algorithms that do not support continuous features (or those that do not handle them well) to work properly. A parameter optimization wrapper allows tuning the parameters of an algorithm automatically based on a search in the parameter space that optimizes the accuracy estimate with different parameters.

The following inducers are created as combinations of others:

IDTM Induction of Decision Tables with Majority. A feature subset selection wrapper on top of decision tables (Kohavi 1995*a*, Kohavi 1995*c*).

C4.5-auto Automatic parameter setting for C4.5 (Kohavi & John 1995).

FSS Naive-Bayes Feature subset selection on top of Naive-Bayes (Kohavi & Sommerfield 1995).

NBTree A decision tree hybrid with Naive-Bayes at the leaves (Kohavi 1996).

The ability to create hybrid algorithms and wrapped algorithms is a very important and powerful approach for multistrategy learning. With $\mathcal{MLC}$++ you do not have to implement two algorithms; you just have to decide on how to integrate them or wrap one around the other.

3.3 $\mathcal{MLC}$++ Utilities

The $\mathcal{MLC}$++ utilities are a set of individual executables built using the $\mathcal{MLC}$++ library. They are designed to be used by end users with little or no programming knowledge. All utilities employ a consistent interface based on options that may be set on the command line or through environment variables.

Several utilities are centered around induction. These are Inducer, AccEst, LearnCurve, and biasVar. Inducer simply runs the induction algorithm of your choice on the dataset, testing the resulting classifier using a test file. AccEst estimates the performance of an induction algorithm on a dataset using any of the accuracy estimation techniques provided (holdout, cross-validation, or bootstrap). LearnCurve builds a graphical representation of the learning curve of an algorithm

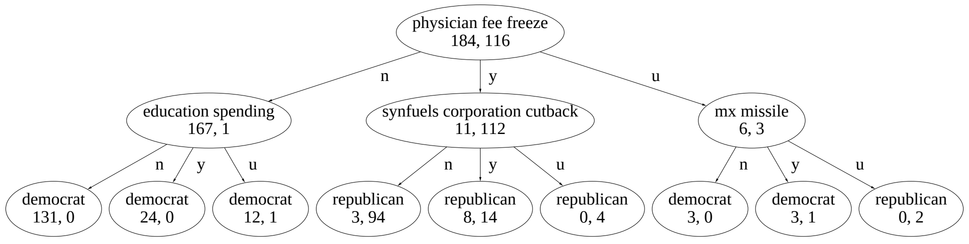


Figure 1: A dot display of a decision tree for the congressional voting dataset.

by running the algorithm on differently sized samples of the given dataset; the output can be displayed using Mathematica or Gnuplot. The biasVar utility provides a bias-variance decomposition of the classification error based on Kohavi & Wolpert (1996).

The remaining utilities provide dataset operations. The Info utility generates descriptive statistics about a dataset, including counts of the number of attributes, class probabilities, and the number of values for each attribute. The Project utility performs the equivalent of a database's SELECT operation, allowing the user to remove attributes from a dataset. The Discretization utility converts real-valued attributes into nominal-valued attributes using any of a number of supervised discretization methods supported by the library. Finally, the Conversion utility changes multi-valued nominal attributes to local or binary encodings which may be more useful for nearest-neighbor or neural-network algorithms.

3.4 Visualization

Some induction algorithms support visual output of the classifiers. All graph-based algorithms support can display two-dimensional representations of their graphs using dot and dotty (Koutsofios & North 1994). Dotty is also capable of showing extra information at each node, such as class distributions. Figure 1 shows such a graph.

The decision tree algorithms, such as ID3, may generate output for Silicon Graphics' MineSet product. The Tree Visualizer provides a three-dimensional view of a decision tree with interactive fly-through capability. Figure 2 shows a snapshot of the display.

$\mathcal{MLC}$++ also provides a utility for displaying General Logic Diagrams from classifiers implemented in $\mathcal{MLC}$++. General Logic Diagrams (GLDs) are graphical projections of multi-dimensional discrete spaces onto two dimensions. They are similar to Karnaugh maps, but are generalized to non Boolean inputs and outputs. A GLD provides a way of displaying up to about ten dimensions in a graphical representation that can be understood by humans. GLDs were described in Michalski (1978) and later used in Wnek, Sarma, Wahab & Michalski (1990), Thrun *et al.* (1991), and Wnek & Michalski (1994) to compare algorithms. They are sometimes called *Dimensional Stacking* (LeBlank, Ward & Wittels 1990) and have been rediscovered many times. Figure 3 shows a GLD for the monk1 problem.

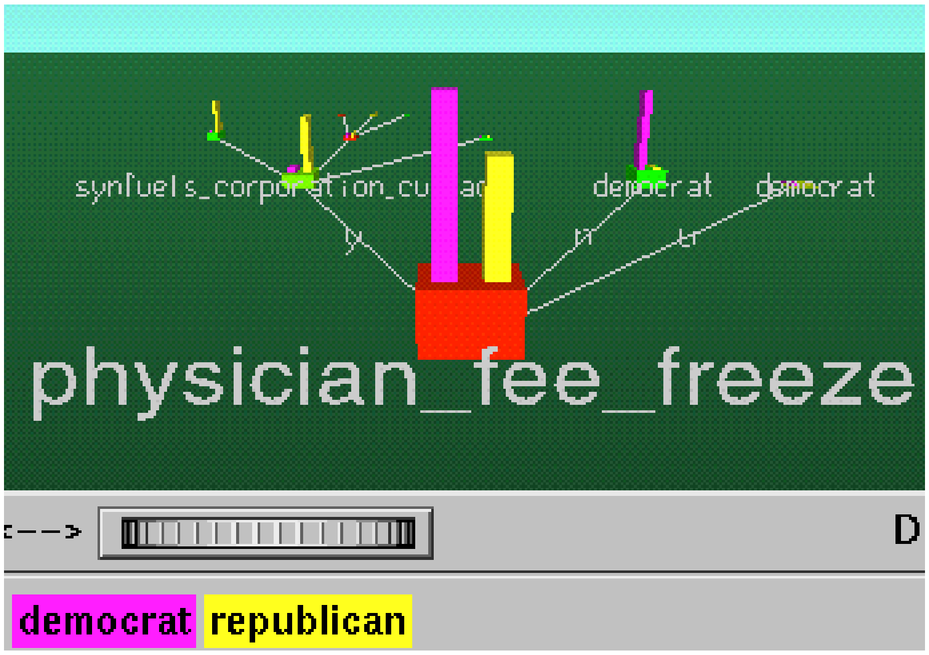


Figure 2: A snapshot of the MineSet Tree Visualizer fly-through for a decision tree.

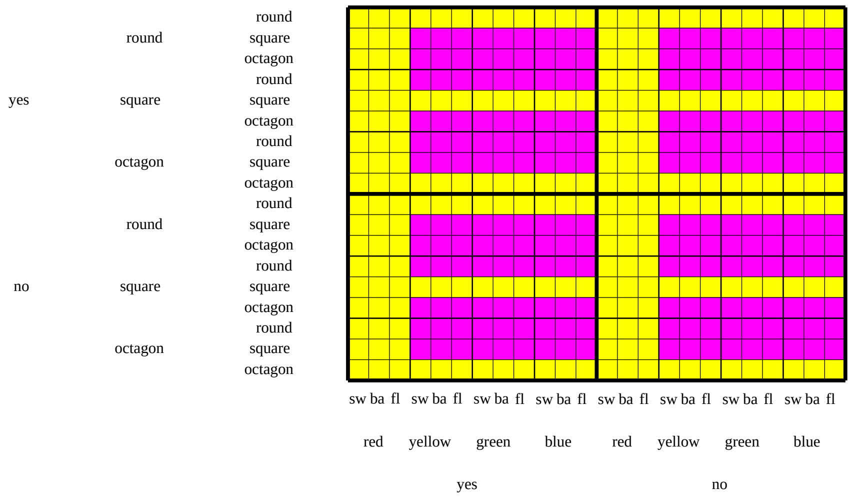


Figure 3: A GLD for the monk1 problem.

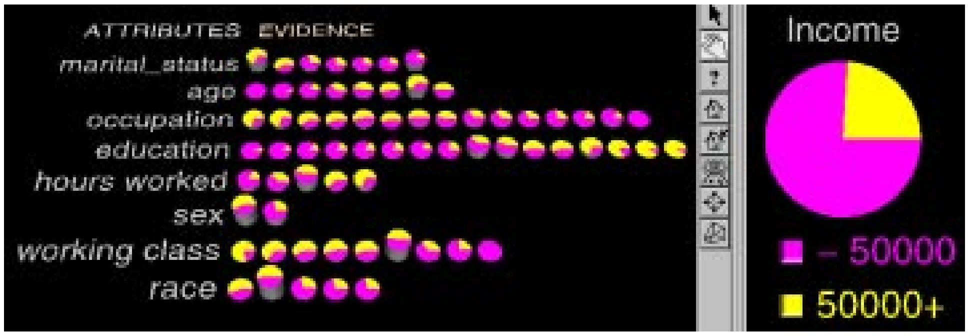


Figure 4: The evidence visualizer's pie-chart display of the Naive-Bayes model. The height of each pie represents the number of instances for that value or range.

Finally, the Naive Bayes algorithm may be visualized two distinct ways, both provided through the Evidence Visualizer utility in MineSet. The first view, in Figure 4, shows straight probabilities as three dimensional pie charts. Each chart represents the distribution of classes given that a single attribute is set to a specific value. The pies are a useful visualization, but their probability values must be multiplied to form the posterior probabilities used for prediction. The second view, in Figure 5, is based on the selection of a single class. The pie charts are replaced by a three dimensional bar chart. The height of each bar represents the log probability (evidence) in favor of the specified class given that a single attribute is set to a specific value. Log probabilities are useful because they may be added to form the posterior, thereby making the Naive Bayes classification process more intuitive.

Both views support interactive classification of data. A single pie chart at the right initially displays the prior class distribution. Users may interact with the visualization by selecting values for the attributes and observing how the posterior probability (pie chart on the right) changes. For example, selecting the pie for *sepal-length* < 5.45 inches and the pie for *sepal-width* > 3.05 inches shows that an iris with these characteristics is probably an iris-setosa (Figure 6). Users can ask questions of the form: "what if I had an instance with certain values" and see the classifier predictions and the posterior probabilities according to the Naive-Bayes model.

3.5 A Global Comparison

Statlog (Taylor, Michie & Spiegalhalter 1994) was a large project that compared about 20 different learning algorithms on 20 datasets. The project, funded by the ESPRIT program of the European Community, lasted from October 1990 to June 1993. Without a tool such as $\mathcal{MLC}$++, an organization with specific domain problems cannot easily repeat such an effort in order to choose the appropriate algorithms. Converting data formats, learning the different algorithms, and running many of them is usually out of the question. $\mathcal{MLC}$++, however, can easily provide such a comparison.

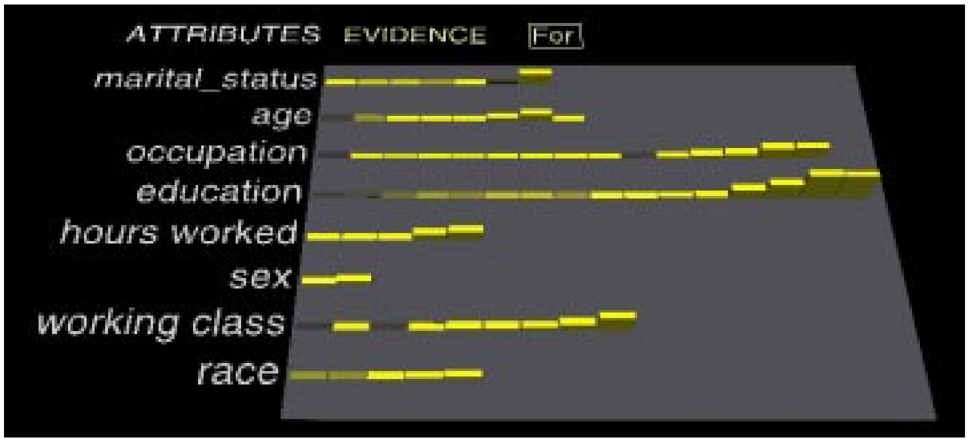


Figure 5: The evidence visualizer's bar-chart display of the Naive-Bayes model. The bars become less saturated as the number of instances decreases, signifying a wider confidence interval.

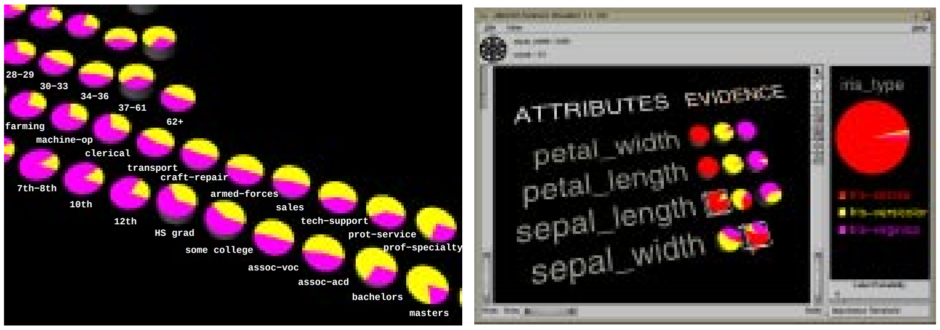


Figure 6: Closeup on some attribute values (left) and selection of specific value ranges to see the posterior probability (right). Users can highlight a pie chart by moving the cursor over it. A message then appears at the top showing the attribute value (or range) and the number of instances having that value (or range). The pie's height is proportional to this number. Pointing to the items in the legend on the right pane, shows the numerical probabilities corresponding to the slice size.

Table 1: The datasets used, the number of attributes, the training and test-set sizes, and the baseline accuracy (majority class).

Dataset	Attributes	Train size	Test size	Majority accuracy
adult	14	30,162	15,060	75.22
chess	36	2,130	1,066	52.22
DNA	180	2,000	1,186	51.91
led24	24	200	3000	10.53
letter	16	15,000	5,000	4.06
shuttle	9	43,500	14,500	78.60
satimage	36	4,435	2,000	23.82
waveform-40	40	300	4,700	33.84

In this section we present a comparison on some large datasets from the UC Irvine repository (C. Blake & Merz 1998). We also take this opportunity to correct some misunderstandings of results in Holte (1993). Table 1 shows the basic characteristics of the chosen domains. Instances with unknown values were removed from the original datasets.

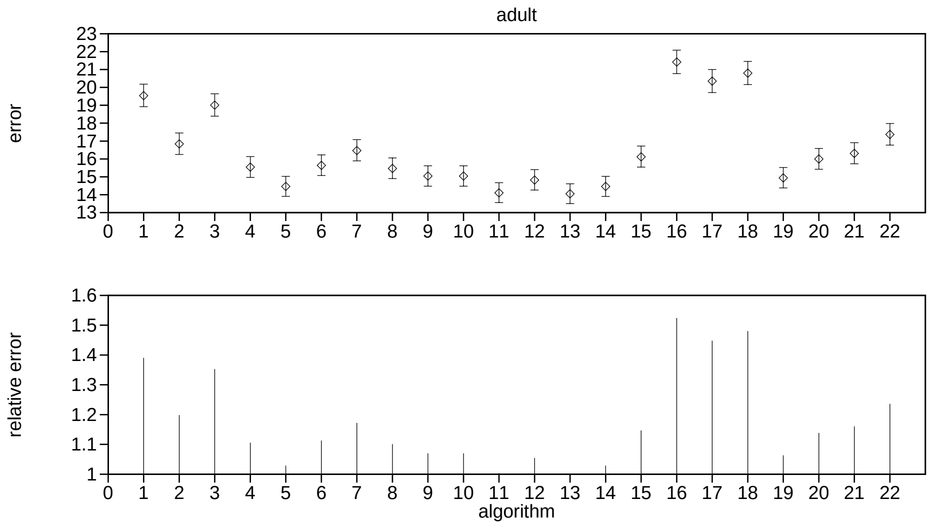
Holte showed that for many small datasets commonly used by researchers in machine learning circa 1990, simple classifiers perform surprisingly well. Specifically, Holte proposed an algorithm called 1R, which learns a complex rule (with many intervals), but using only a single attribute. He claimed that such a simple rule performed surprisingly well. On sixteen datasets from the UCI repository, the error rate of 1R was 19.82% while that of C4.5 was 14.07%, a difference of 5.7%.

While it is surprising how much one can do with a single attribute, a different way to look at this result is to look at the *relative error*, or the increase in error of 1R over C4.5. This increase is over 40%, which is very significant if an organization has to pay a large amount of money for every mistake made.

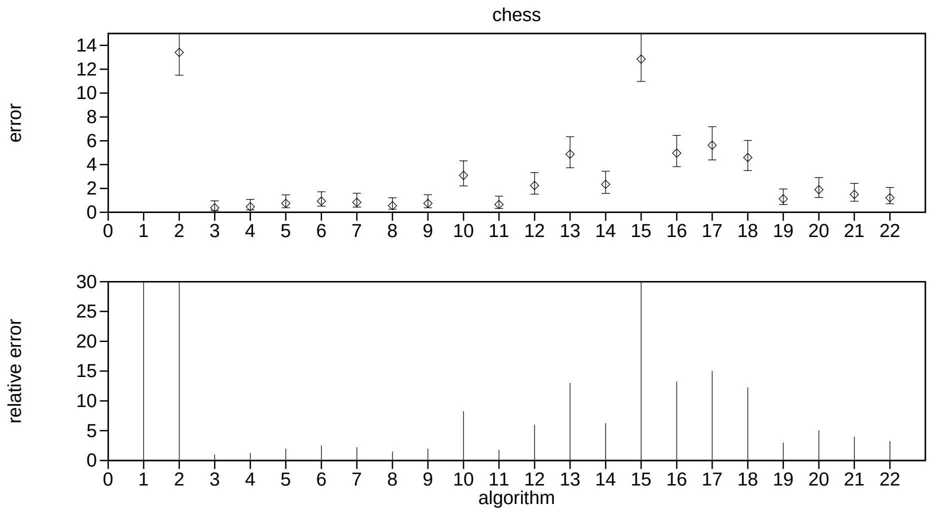
Figures 7 to 10 show a comparison of 22 algorithms on eight large datasets from the UC Irvine repository. The Aspirin/MIGRAINES neural-network did not converge on letter and adult and we took the saved model after 60 hours or running time on an SGI Origin 2000.

Our results show that for different domains different algorithms perform differently and that there is no single clear winner. However, they also show that for the larger real-world datasets at UC Irvine, some algorithms are generally safe-bets and some are pretty bad in general. Specifically, algorithms 5 (C4.5-auto), 6 (Voted ID3 0.6), 7 (Voted ID3 0.8), 8 (Bagging ID3), 9 (Option Decision Trees), 11 (NBTree), and 13 (FSS Naive-Bayes) were among the best performers in at least three out of the eight datasets, while algorithms 1 (1R), 2 (T2) were consistently worst performers. In fact, 1R was in the worst set in seven out of eight datasets and T2 was in the worst set in four out of eight datasets and could not even be run on two other datasets because it required over 512MB of memory.

While there is very little theory on how to select algorithms in advance, simply running many algorithms and looking at the output and accuracy is a practical



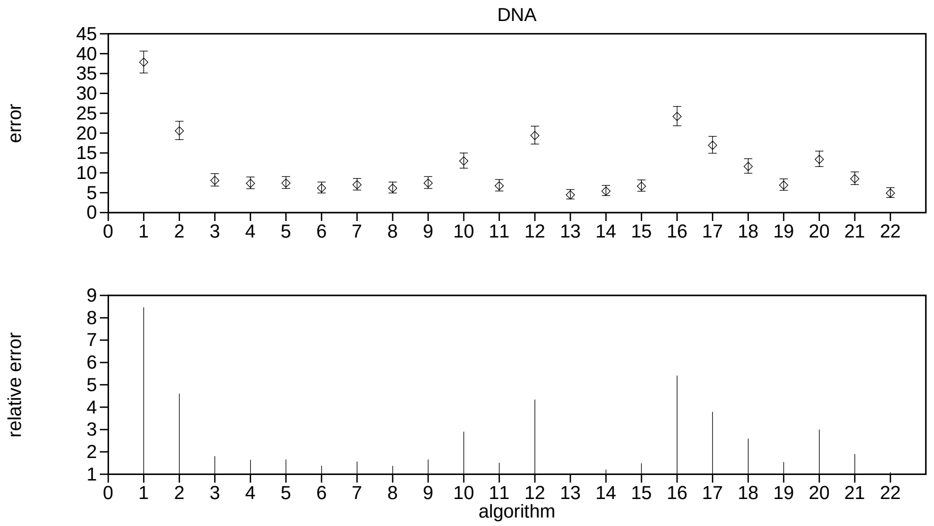
Best algorithms: 5,11,13,14, worst algorithms: 16,17,18



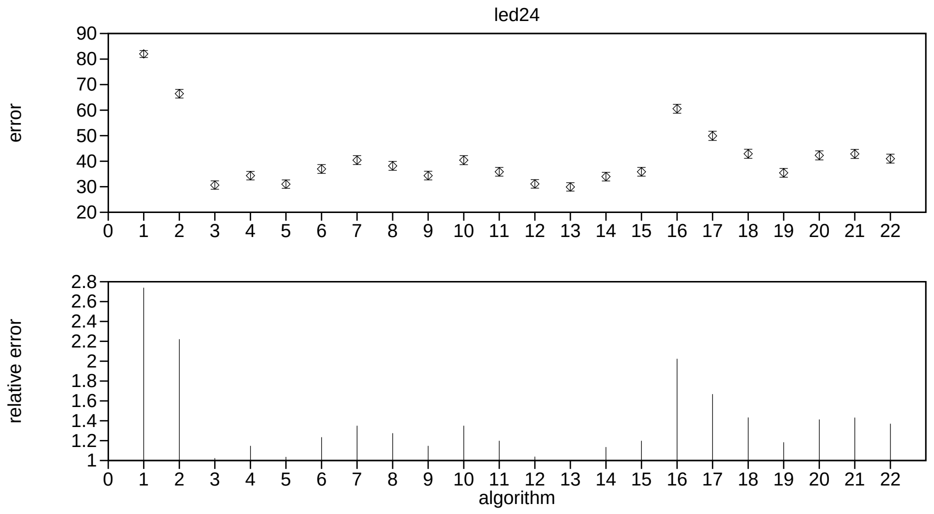
Best algorithms: 3,4,5,6,7,8,9,11, worst algorithms: 1,2,15

1	1R	2	T2	3	CART
4	C4.5	5	C4.5-auto	6	Voted ID3 (0.6)
7	Voted ID3 (0.8)	8	Bagging ID3	9	Option trees
10	OC1	11	NBTree	12	HOODG
13	FSS Naive Bayes	14	IDTM (Decision table)	15	Naive-Bayes
16	Nearest-neighbor (1)	17	Nearest-neighbor (3)	18	PEBLS
19	C4.5 rules	20	CN2	21	Ripper
22	NN-AM				

Figure 7: Error and relative errors for the learning algorithms.



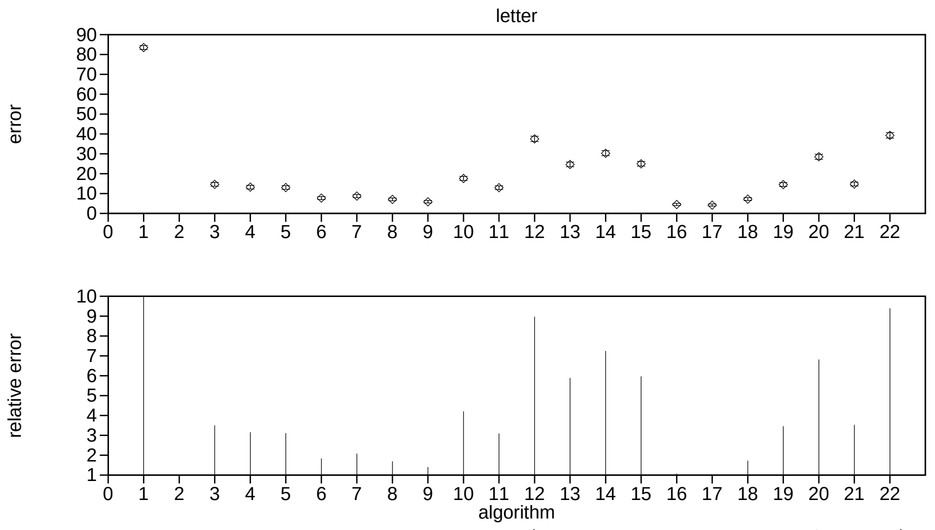
Best algorithms: 13,14,22, worst algorithms: 1,2,12,16



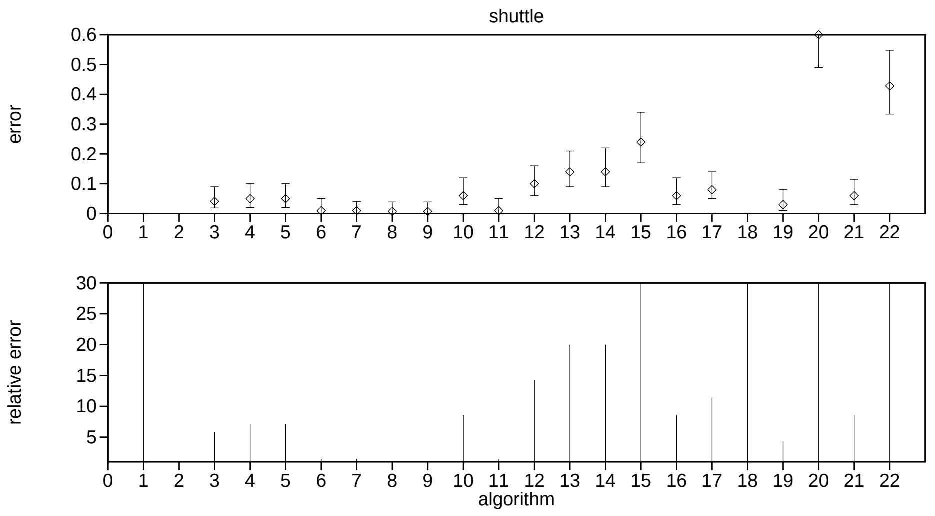
Best algorithms: 3,5,12,13, worst algorithms: 1,2,16

1	1R	2	T2	3	CART
4	C4.5	5	C4.5-auto	6	Voted ID3 (0.6)
7	Voted ID3 (0.8)	8	Bagging ID3	9	Option trees
10	OC1	11	NBTree	12	HOODG
13	FSS Naive Bayes	14	IDTM (Decision table)	15	Naive-Bayes
16	Nearest-neighbor (1)	17	Nearest-neighbor (3)	18	PEBLS
19	C4.5 rules	20	CN2	21	Ripper
22	NN-AM				

Figure 8: Error and relative errors for the learning algorithms.



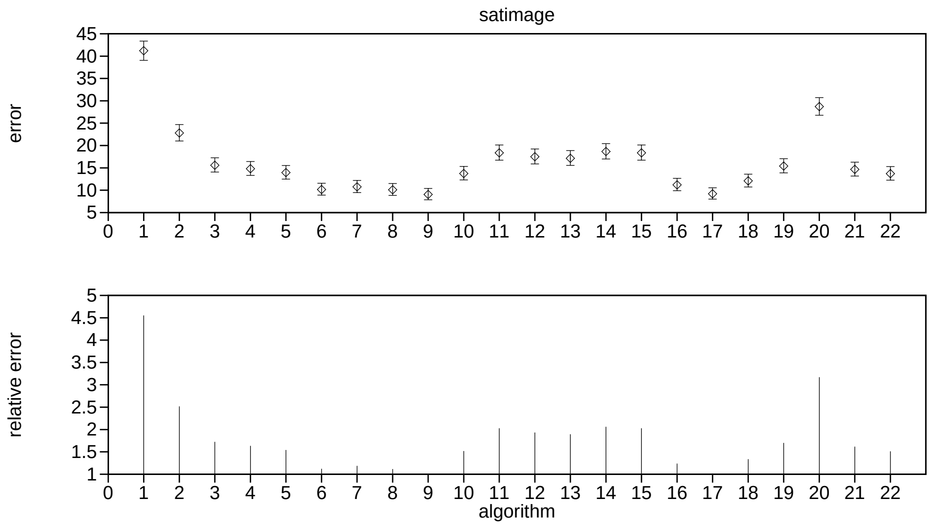
Best algorithms: 16,17, worst algorithms: 1,2,12,22 (2 needed more than 512MB of memory)



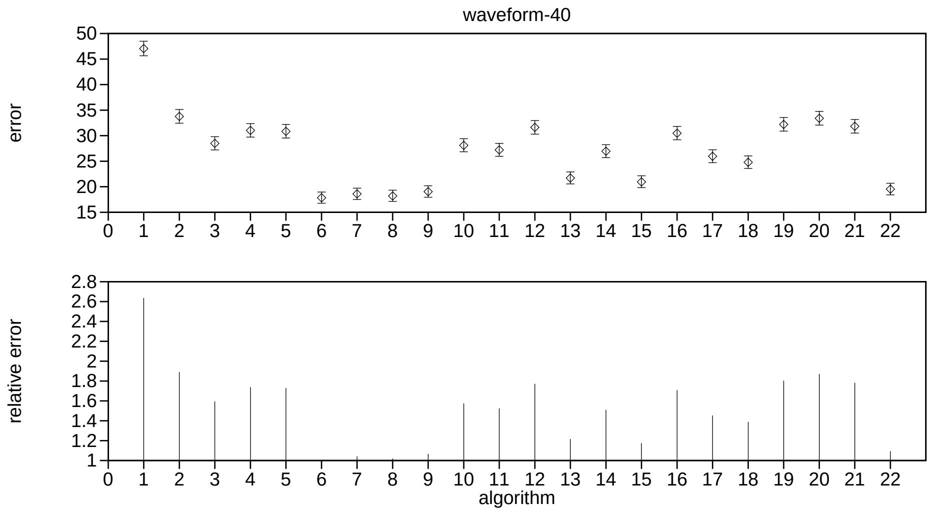
Best algorithms: 6,7,8,9,11,19, worst algorithms: 1,2,3,15,18,20,22 (some not shown because they are out of range. Algorithm 1=5.32%, 2=not enough memory, 3=7.5%, 18=23.6%)

1	1R	2	T2	3	CART
4	C4.5	5	C4.5-auto	6	Voted ID3 (0.6)
7	Voted ID3 (0.8)	8	Bagging ID3	9	Option trees
10	OC1	11	NBTree	12	HOODG
13	FSS Naive Bayes	14	IDTM (Decision table)	15	Naive-Bayes
16	Nearest-neighbor (1)	17	Nearest-neighbor (3)	18	PEBLS
19	C4.5 rules	20	CN2	21	Ripper
22	NN-AM				

Figure 9: Error and relative errors for the learning algorithms. T2 (2) needed over 512MB of memory for the letter and shuttle datasets.



Best algorithms: 6,8,9,17, worst algorithms: 1,20



Best algorithms: 6,7,8, worst algorithms: 1,2,20

1	1R	2	T2	3	CART
4	C4.5	5	C4.5-auto	6	Voted ID3 (0.6)
7	Voted ID3 (0.8)	8	Bagging ID3	9	Option trees
10	OC1	11	NBTree	12	HOODG
13	FSS Naive Bayes	14	IDTM (Decision table)	15	Naive-Bayes
16	Nearest-neighbor (1)	17	Nearest-neighbor (3)	18	PEBLS
19	C4.5 rules	20	CN2	21	Ripper
22	NN-AM				

Figure 10: Error and relative errors for the learning algorithms.

solution with $\mathcal{MLC}$++.

4 $\mathcal{MLC}$++ for Software Developers

If you want to write an efficient C++ program, you must first be able to write an efficient program*... micro-tuning leads nowhere if the higher-level algorithms you employ are inherently inefficient. Do you use quadratic algorithms when linear ones are available?... If so, you can hardly be surprised if your programs are described like second-rate tourist attractions: worth a look, but only if you've got some extra time.*
—Meyers (1996)

$\mathcal{MLC}$++ source code is public domain, including all the sources. $\mathcal{MLC}$++ contains over 60,000 lines of code and 14,000 lines of regression testing code. The $\mathcal{MLC}$++ utilities are only 2,000 lines of code that use the library itself.

One of the advantages of using $\mathcal{MLC}$++ for software developers is that it provides high-quality code and encourages high-quality code development. By providing a large number of general purpose classes as well as a large set of classes specific to machine learning, $\mathcal{MLC}$++ ensures that coding remains a small part of the development process. Mature coding standards and a shallow class hierarchy insure that new code is robust and helpful to future developers. Although it can take longer to write fully-tested code using $\mathcal{MLC}$++, ultimately, $\mathcal{MLC}$++ greatly decreases the time needed to complete a robust product.

$\mathcal{MLC}$++ includes a library of general purpose classes, independent of machine learning, called MCore. MCore classes include strings, lists, arrays, hash tables, and input/output streams, as well as some built-in mechanisms for dealing with C++ initialization order, options, temporary file generation and cleanup, as well as interrupt handling. MCore classes not only provide a wide range of functions, they provide solid tests of these functions, reducing the time it takes to build more complex operations. All general-purpose classes used within the full library are from MCore, with the exception of graph classes from the LEDA library (Naeher 1996). Although the classes in MCore were built for use by the $\mathcal{MLC}$++ library, they are not tied to machine learning and may be used as a general purpose library. MCore is a separate library which may be linked independently of the whole library.

$\mathcal{MLC}$++ classes are arranged more or less as a library of independent units, rather than as a tree or forest of mutually-referent set of modules requiring multiple link and compile stages. The ML and MInd modules follow this philosophy by providing a series of classes which encapsulate basic concepts in machine learning. Inheritance is only used where it helps the programmer. By resisting the temptation to maximize use of C++ objects, we were able to provide a set of basic classes with clear-cut interfaces for use by anyone developing a machine learning algorithm.

The important concepts provided by the library include Instance lists, Categorizers (classifiers), Inducers, and Discretizers. Instance lists and supporting classes hold the database on which learning algorithms are run. Categorizers (also known as classifiers) and Inducers (induction algorithms) represent the algorithms themselves: an Inducer is a machine learning algorithm that produces a classifier that, in turn, assigns a class to each instance. Discretizers replace real-valued attributes in the database with discrete-valued attributes for algorithms which can only use discrete values. $\mathcal{MLC}$++ provides several discretization methods (Dougherty, Kohavi & Sahami 1995, Kohavi & Sahami 1996).

Programming with $\mathcal{MLC}$++ generally requires little coding. Because $\mathcal{MLC}$++ contains many well-tested modules and utility classes, the bulk of $\mathcal{MLC}$++ programming is determining how to use the existing code base to implement new functionality. Although learning how to use a large code base takes time, we now find that the code we write is much easier to test and debug because we can leverage the testing and debugging done on the rest of the library. Additionally, forcing the developer to break a problem down into $\mathcal{MLC}$++ concepts insures that $\mathcal{MLC}$++ maintains its consistent design, which in turn insures consistent code quality.

Each class in $\mathcal{MLC}$++ is testable almost independently with little reliance on other classes. We have built a large suite of regression tests to insure the quality of each class in the library. The tests will immediately determine if a code change has created a problem. The goal of these tests is to force bugs to show up as close to their sources as possible. Likewise, porting the library is greatly simplified by these tests, which provide a clear indication of any problems with a port. Unfortunately, many C++ compilers still do not support full ANSI C++ templates that are required to compile $\mathcal{MLC}$++.

One problem with C++ is the temptation to create complex class hierarchies simply because it is possible. In hindsight, we learned that such hierarchies hinder the library's main goals of usability and robustness. For example, the InstanceList class used to be eight individual classes, depending on whether or not the list was ordered, whether or not the list kept statistical information, and whether or not the instances in the list were labelled. Although these are all important abstract distinctions between different types of instance lists, making them separate classes turned out to be less useful and more error prone than having a single "smart" InstanceList class that, for example, provides statistical information on the fly using caching schemes.

5 $\mathcal{MLC}$++ Development in Hindsight

Hindsight is always twenty-twenty
—Billy Wilder

Many decisions had to be made during the development of $\mathcal{MLC}$++. We tackled such issues as which language to use, what libraries, whether users must know how to code in order to use it, and how much to stress efficiency versus safety.

We decided that $\mathcal{MLC}$++ should be useful to end-users who have neither programmed before nor want to program now (many lisp packages for machine learning require writing code just to load the data). We realized that a GUI would be very useful; however, we concentrated on adding functionality, providing only a simple but general environment variable-based command-line interface. We also provided the source code for other people to interface. $\mathcal{MLC}$++ was used to teach machine learning courses at Stanford and many changes to the library were made based on student's feedback.

We chose C++ for a number of reasons. First, C++ is a good general-purpose language; it has many useful features but imposes no style requirements of its own. Features such as templates allowed us to maintain generality and reusability along with the safety of strong typing and static checking. Second, the language's object-oriented features allowed us to decompose the library into a set of modular objects which could be tested independently. At the same time, C++'s relative flexibility allowed us to avoid the object-oriented paradigm when needed. Third, C++ has no language-imposed barriers to efficiency; functions can be made inline, and objects and be placed on the stack for faster access. This gave use the ability to optimize code in critical sections. Finally, C++ is a widely accepted language which is gaining popularity quickly. Since the project was created at Stanford, it was extremely useful to use a language which everybody wanted to learn and use.

We also made a decision to use the best compiler we found at the time (CenterLine's ObjectCenter) and to use all available features. We assumed that GNU's g++ compiler would catch up. In 1987 "Mike Tiemann gave a most animated and interesting presentation of how the GNU C++ compiler he was building would do just about everything and put all other C++ compiler writers out of business" (Stroustroup 1994). Sadly, the GNU C++ compiler is still weaker than most commercial grade compilers and (at least as of 1995) cannot handle templates well enough. Moreover, most PC-based compilers still cannot compile $\mathcal{MLC}$++. We hope that this will change as 32-bit operating systems mature and compilers improve.

We quickly chose LEDA (Naeher 1996) for graph manipulation and algorithms, and GNU's libg++, which provided some basic data structures. Unfortunately, the GNU library was found to be deficient in many respects. It hasn't kept up with the emerging C++ standards (*e.g.*, constness issues, templates) and we slowly rewrote all the classes used. Today $\mathcal{MLC}$++ does not use libg++. If we were starting the project today, we would likely use the C++ Standard Template Library (STL), since it provides a large set of solid data structures and algorithms, has the static safety of templates, and is likely to be a widely accepted standard. One current disadvantage of many class libraries, including $\mathcal{MLC}$++, is that developers must learn a large code base of standard data structures and algorithms. This greatly increases the learning curve to use the library. Use of a standard library like STL might flatten that curve.

Much of what was done in $\mathcal{MLC}$++ was motivated by research interests of the first author. This resulted in a skewed library with many symbolic algorithms and no work on neural networks nor any statistical regression algorithms. Neural network and statistical algorithms were also shunned because many such algorithms already existed and there seemed to be little need to write yet another one when it would not contribute to immediate research interests. However, today, with the focus shifting toward data mining, the library is becoming increasingly more balanced.

6 Related Work

Several large efforts have been made to describe data mining algorithms for knowledge discovery in data. We refer the reader to the URL

`http://www.kdnuggets.com/siftware.html` for pointers and description. Additionally, an excellent comparison of commercial data mining tools is available from Two Crows (Brand, Edelstein, Gerritsen, Millenson, Schubert, Small & Small 1997), and a slightly outdated report is available from Intelligent Software Strategies (Hall 1996). Typical features of commercial products include classification (decision trees, neural networks, instance-based methods), clustering, regression, pattern detection, and associations.

SGI's MineSet MineSet is Silicon Graphics' data mining and visualization product. From release 1.1 and on, it uses $\mathcal{MLC}$++ as a base for the induction and classification algorithms. Classification models built are either shown using the 3D visualization tools or used for prediction. MineSet has a GUI interface and accesses commercial databases including Oracle, Sybase, and Informix using a client/server architecture. Besides classification, MineSet also provides an association algorithm, automatic binning of real-valued data, and a feature selection algorithm.

ISL's Clementine Clementine includes a neural network and an interface to C4.5 for decision tree and rule induction. It has a strong dataflow-based GUI and simple visualizations.

IBM's Intelligent Miner IBM's Intelligent Miner provides a variety of knowledge discovery algorithms for classification, associations, clustering, deviation detection, and sequential pattern discovery. Some of the algorithms in Intelligent Miner scale to large datasets.

SAS SAS provides a huge variety of statistical and data mining tools, including neural network, decision trees, discriminant analysis, logistic regression, and visualization.

Angoss's KnowledgeSeeker Angoss provides a decision tree induction system with visualization.

HNC's Marksman HNC provides neural network technology for classification, clustering, and visualization. It comes with a PC SNAP board containing 16 parallel processors.

TMC's Darwin Darwin is a suite of learning tools developed by Thinking Machines. It is intended for use on large databases and uses parallel processing for speedup. Its algorithms include Classification and Regression Trees (CART), Neural networks, Nearest Neighbor, and Genetic Algorithms. Darwin also includes some 2D visualization.

NeoVista NeoVista Decision Series provides an integrated suite of mining tools for use with large databases and legacy systems. Discovery methods used include nerual networks, clustering, genetic algorithms, and association rules. NeoVista focuses heavily on model deployment in decision support systems and provides consulting services along with the software.

NeuralWare's NeuralWorks NeuralWare provide neural-network technology for classification, clustering, regression, and time-series prediction.

DataMind DataMind DataCruncher is a client/server system for mining data from data warehouses and data marts. DataMind supports proprietary agent network technology for classification.

HyperParallel HyperParallel provides several data mining algorithms including classification, clustering, and associations. The tools are parallelized and can analyze very large business problems.

Unica Unica provides PRW, a Pattern Recognition Workbench, which was designed to solve statistical and pattern recognition problems. It is a complete integrated environment and supports classification, clustering, time series, and regression.

Modelware Modelware is a commercial datamining tool including classification using a nearest neighbor algorithm along with a proprietary process modeling algorithm. Modelware also includes a GUI and basic visualization.

DataEngine DataEngine is an integrated data analysis tool which uses fuzzy logic, nerual networks, and statistical methods to implement a number of discovery tasks such as classification, clustering, dependency analysis, and function approximation. It also provides basic data acquisition and visualization.

The Data Mining Suite The Data Mining Suite from Information Discovery is a set of products encompassing several discovery operations. The product supports prediction based on rules, patterns, and anomolies in data. Methods supported are classification, clustering, summarization, deviation detection, dependency analysis, and geographic pattern discovery.

Partek Partek provides data mining and knowledge discovery software using a number of tools and techniques. These include classification, clustering, function approximation, principal components analysis, multi-dimensional scaling, correspondence analysis, and variable selection. Partek employs statistical methods along with neural networks and genetic algorithms.

ModelQuest ModelQuest is a set of data mining tools including algorithms for classification, summarization, deviation detection, dependency analysis, geographic discovery, fault detection, fraud detection, prediction, and estimation. The system uses a combined statistical/ neural network approach and includes substantial automation to free the user from parameter tuning.

XpertRule Analyser XpertRule Analyser is an integrated data mining tool. Strategies include classification, rule induction, neural networks, and genetic algorithms.

In addition to the many commercial systems, a number of research tools exist. Some of these have goals similar to $\mathcal{MLC}$++.

Kepler Kepler is an extensible data mining/machine learning system developed at GMD. It allows addition of new algorithms through a plug-in approach. Kepler currently provides plug-ins to support decision tree induction, backprop neural networks, pattern detection, clustering, nearest neighbor learning, multiple adaptive regression splines, and first-order learning tools. Additionally, Kepler supports database operations such as aggregation and sampling.

WEKA WEKA, or Waikato Environment for Knowledge Analysis, is a software workbench for application of machine learning. It provides a uniform user interface as well as a number of different algorithms, including rule induction (1R, T2, and Induct), Instance based learning (IB1-4, PEBLS, and K*), Regression (M5'), and Relational rules (FOIL). It also provides an interface to several external algorithms (C4.5, Classweb, and a better rule evaluator).

MLToolbox MLToolbox is a collection of many publicly available algorithms and re-implementations of others. The algorithms do not share common code and interface.

TOOLDIAG TOOLDIAG is a collection of methods for statistical pattern recognition, especially classification. While it contains many algorithm, such as k-nearest neighbor, radial basis functions, parzen windows, feature selection and extraction, it is limited to continuous attributes with no missing values.

Mobal Mobal is a multistrategy tool which integrates manual knowledge acquisition techniques with several automatic first-order learning algorithms. The entire system is rule-based and existing knowledge is stored using a syntax similar to predicate logic.

Emerald Emerald is a research prototype from George Mason University. Its main features are five learning programs and a GUI. The lisp-based system is capable of learning rules which are then translated to English and spoken by a speech synthesizer. The algorithms include algorithms for learning rules from examples, learning structural descriptions of objects, conceptually grouping objects or events, discovering rules characterizing sequences, and learning equations based on qualitative and quantitative data.

Sipina-W Sipina-W is a machine learning and knowledge engineering tool package which implemented CART, ID3, C4.5, Elisee (segmentation), Chi^{2}Aid, and SIPINA algorithms for classification. Sipina-W runs on real or discrete-valued data sets and is oriented toward the building and testing of expert systems. It reads ASCII, dBase, and Lotus format files.

Brute Brute is an inductive learning system for performing classification and machine learning using several well known algorithms (BruteDL, Greedy3, Kdl, 1R) and variations thereof. It uses a massive search strategy as opposed to greedy search.

DBMiner DBMiner is a semi-commercial integrated system for finding multiple-level knowledge in large relational databases. It is an updated version of an earlier system called DBLearn. The system applies an attribute-oriented induction method. It also provides interactive methods through a user-friendly interface.

7 Summary

$\mathcal{MLC}$++, a Machine Learning library in C++, has greatly evolved over the last three years. It now provides developers with a substantial piece of code that is well-organized into a useful C++ hierarchy. Even though (or maybe because) it was mostly a research project, we managed to keep the code quality high with many regression tests.

The library provides end-users with the ability to easily test-drive different induction algorithms on datasets of interest. Accuracy estimation and visualization of classifiers allow one to pick the best algorithm for the task.

Silicon Graphics new data mining product, MineSet 1.1, has classifiers built on top of $\mathcal{MLC}$++ with a GUI and interfaces to commercial databases. We hope this will open machine learning and data mining to a wider audience.

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A Review of Some Theoretical Results

Over the years, many properties of classification algorithms have been proved. For example, Fix & Hodges (1951) developed the consistency properties of nearest-neighbor procedures and showed that these procedures have asymptotically optimum properties for large sample sets. Cover & Hart (1967) showed that that the error of one-nearest-neighbor is asymptotically at most twice the Bayes error (best possible error), implying that half of all the information in an infinite sample is contained in a single nearest neighbor. Dasarathy (1990) provides an excellent review of nearest-neighbor algorithms. Gordon & Olshen (1978, 1984) showed sufficient conditions for decision-tree induction algorithms to be asymptotically Bayes risk efficient.

While asymptotic consistency results are comforting because they guarantee that with enough data the learning algorithms will converge to the target concept one is trying to learn, our world is not so ideal. We are always given finite amounts of data from which to learn and rarely do we reach asymptopia.[1]

Soon after the original paper by Fix & Hodges, the authors evaluated the performance of nearest-neighbors on small samples (Fix & Hodges 1952); the differences were very significant. All common decision-tree implementations, such as CART (Breiman et al. 1984), ID3 (Quinlan 1986), and C4.5 (Quinlan 1993), are not known to be consistent. For example, none of them make the random splits that Gordon & Olshen (1978) show is a sufficient condition for consistency (although this is not known to be a necessary condition).

From a theoretical standpoint, the no-free-lunch theorems and the conservation law (Wolpert 1994, Schaffer 1994) show that for a finite dataset size and discrete inputs (or finite precision floating point numbers), no algorithm can outperform any other on average if all target concepts are equally probable.

Authors have recently claimed some "surprising" results about oversearching. For example, Murphy & Pazzani (1994) showed that the smallest trees are not always the best predictors. Quinlan (1995) discusses oversearching and how it can hurt performance. Murthy & Salzberg (1995) showed how too much lookahead can also hurt performance. These can be explained with the bias-variance decomposition of error.

The bias-variance decomposition of error (Geman, Bienenstock & Doursat 1992, Kohavi & Wolpert 1996, Breiman 1996*a*) shows how to decompose the error of learning algorithms into two components: the bias, which measure how closely the learning algorithm's average guess (over all possible training sets of the given training set size) matches the target; and the variance, which measures how much the learning algorithm's guess varies (bounces around) for the different training sets of the given size. While most of our intuition is geared at reducing the bias and making the algorithm able to fit the targets better, the variance component is sometimes the dominant factor and is now getting more attention from the community (Breiman 1994).

[1]Pun on utopia intended.