

To the Graduate Council:

I am submitting herewith a thesis written by Isaac Sherman entitled "On the Role of Genetic Algorithms in the Pattern Recognition Task of Classification." I have examined the final paper copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Computer Science.

Bruce MacLennan, Major Professor

We have read this thesis
and recommend its acceptance:

Dr. Bruce MacLennan

Dr. Hairong Qi

Dr. Catherine Schuman

Accepted for the Council:

Dixie L. Thompson

Vice Provost and Dean of the Graduate School

To the Graduate Council:

I am submitting herewith a thesis written by Isaac Sherman entitled "On the Role of Genetic Algorithms in the Pattern Recognition Task of Classification." I have examined the final electronic copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Computer Science.

Bruce MacLennan, Major Professor

We have read this thesis
and recommend its acceptance:

Dr. Bruce MacLennan

Dr. Hairong Qi

Dr. Catherine Schuman

Accepted for the Council:

Dixie L. Thompson

Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)

On the Role of Genetic Algorithms in the Pattern Recognition Task of Classification

A Thesis Presented for
The Master of Science
Degree

The University of Tennessee, Knoxville

Isaac Sherman

May 2017

© by Isaac Sherman, 2017
All Rights Reserved.

To Shannon, David, and Zach. You know what you did.

Acknowledgements

I would like to thank my graduate committee for their support and help in this project. I'd also like to thank Mark Slep and Joe Vrba, without whom the necessary research never would have taken place. I want to thank Dr. Catherine Schuman for her inspiring me to pursue evolutionary computation. I would like to thank Dr. Hairong Qi for her support and for teaching me everything I never wanted to know about Bayes' rule. I want to thank Dr. Bruce MacLennan for being a patient, great advisor- he's everything a professor should be.

I want to thank my graduate discussion group for their insights and patience with my derailing of the meetings into weird philosophical tangents: Dr. Zahra Mahoor, Alan McBride, Casey Miller, Aaron Mishtal, Todd Young, Jonathon Ferrell, Camille Crumpton, and Andrew August. You were the highlight of my week for most of my time as a graduate student, and without the public shaming of my peers I don't know how much of this work would have ever been completed.

I'd like to thank my family for their support of and patience with me. In general, not just during grad school. Thank you Monica and Darlene LaVerdure for all your help with everything in the past two years. Thank you Anna and Daniel Fredette for helping keep my kid occupied on the weekends. Thanks to my Mom and Sarah for listening to me complain about technical details you couldn't have possibly understood but for letting me work the problem out with you.

Lastly, but certainly not least, let me thank David and Zach for not being too terribly difficult to parent, and thank you Shannon for being amazing in every way.

Beep boop son, beep boop

Abstract

In this dissertation we ask, formulate an apparatus for answering, and answer the following three questions: Where do Genetic Algorithms fit in the greater scheme of pattern recognition? Given primitive mechanics, can Genetic Algorithms match or exceed the performance of theoretically-based methods? Can we build a generic universal Genetic Algorithm for classification? To answer these questions, we develop a genetic algorithm which optimizes MATLAB classifiers and a variable length genetic algorithm which does classification based entirely on boolean logic. We test these algorithms on disparate datasets rooted in cellular biology, music theory, and medicine. We then get results from these and compare their confusion matrices. For those unfamiliar with Genetic Algorithms, we include a primer on the subject in chapter 1, and include a literature review and our motivations. In Chapter 2, we discuss the development of the algorithms necessary as well as explore other features necessitated by their existence. In Chapter 3, we share and discuss our results and conclusions. Finally, in Chapter 4, we discuss future directions for the corpus we have developed.

All code and supporting results can be found at <https://github.com/IsaacSherman/Thesis>.

Contents

List of Tables	ix
List of Figures	xi
1 Introduction	1
2 Methods and Implementations	18
2.1 Overview	18
2.2 Preprocessing	19
2.3 Hybrid Approach	23
2.4 Purist Approach	33
3 Results	46
3.1 Datasets	47
3.2 Results	51
3.2.1 Yeast	51
3.2.2 Cardiotocography NSP	55
3.2.3 Cardiotocography Morphology	57
3.2.4 Bach’s Chorales	59
3.3 Final Thoughts	66
4 Conclusions	68
Bibliography	71

A Hunter Genomes and Explanations	78
A.1 Yeast	78
Vita	86

List of Tables

2.1	Interpretation of Affinity Bits	40
2.2	Merger Outcomes	41
3.1	Yeast: Classification Tree without Feature Selection Confusion Matrix	52
3.2	Yeast: Classification Tree with Feature Selection Confusion Matrix . .	53
3.3	Yeast: Multiclass Naïve Bayes without Feature Selection Confusion Matrix	53
3.4	Yeast: Multiclass Naïve Bayes with Feature Selection Confusion Matrix	54
3.5	Yeast: Hunter	55
3.6	Cardiotocography NSP: Classification Tree without Feature Selection Confusion Matrix	55
3.7	Cardiotocography NSP: Classification Tree with Feature Selection Confusion Matrix	56
3.8	Cardiotocography NSP: Multiclass Naïve Bayes without Feature Selec- tion Confusion Matrix	56
3.9	Cardiotocography NSP: Multiclass Naïve Bayes with Feature Selection Confusion Matrix	57
3.10	Cardiotocography NSP: Hunter Confusion Matrix	57
3.11	Cardiotocology Morphology: Classification Tree Confusion Matrix . .	58
3.12	Cardiotocology Morphology: Classification Tree Confusion Matrix . .	59
3.13	Cardiotocography Morphology: Naïve Bayes without Feature Selection Confusion Matrix	59

3.14	Cardiotocography Morphology: Naïve Bayes without Feature Selection	
	Confusion Matrix	61
3.15	Cardiotocography Morphology: Hunter Confusion Matrix	61

List of Figures

1.1 Basic GA	2
1.2 Roulette Uniform Selection	5
1.3 Mutation	6
2.1 Overall Program Flow	19
2.2 Cardio Config File	20
2.3 Evolver Algorithm	30
2.4 Purist Voting Algorithms	35
2.5 Hunter Crossover	37
2.6 Chromosome Crossover	38
2.7 Daedalus Generate Next Generation	42
3.1 T-SNE visualization of Yeast dataset	49
3.2 T-SNE visualization of Cardio dataset, NSP	50
3.3 T-SNE visualization of Cardio dataset, morphology	51
3.4 T-SNE visualization of Bach dataset	52
3.5 Bach's Chorales Classification Tree Without Feature Selection	60
3.6 Bach's Chorales Classification Tree with Feature Selection	62
3.7 Bach's Chorales Naïve Bayes without Feature Selection	63
3.8 Bach's Chorales Naïve Bayes with Feature Selection	64
3.9 Bach's Chorales Hunter	65
3.10 Hunter Population Growth, CardioNSP	67

3.11 Multiclass Naïve Bayes Optimizer Growth, CardioNSP	67
A.1 Best Hunter, Yeast	80

Chapter 1

Introduction

A Genetic Algorithm (GA) is a biologically inspired form of computing. GAs can be used for many different purposes, from optimization to classification to design and testing. They can be applied anywhere that a solution can be encoded and then autonomously evaluated. However, they are most well understood as a general solution to optimization as a form of stochastic gradient descent, similar conceptually to simulated annealing. In this paper, I attempt to narrow the role of GAs as they pertain to pattern recognition and classification. In the remainder of this chapter I will describe GAs in general terms and discuss the motivations of this paper. In chapter 2, I will discuss the specifics of the GAs which I use in this paper in detail. In chapter 3 I will describe the experiments conducted and discuss the results. In Chapter 4 I will describe future avenues of study which are available.

Genetic Algorithms Introduction Imagine a colony of rabbits. The rabbits are quite content to munch on clovers and thistles and the like. Some rabbits are much more content than others, and have significant girth. One day foxes find the rabbits. There are many more rabbits than foxes, and the foxes can't eat all of them. The heaviest rabbits are both the slowest and the most appetizing to the foxes, and they are the first to go, but many die. They have failed the evolutionary filtering process. However, the rabbits that survive are thinner, and the most successful are

likely faster. These are the rabbits which survive to populate the next generation. GAs encapsulate this process, though usually with much less mayhem. The algorithm is as follows:

1.1: Basic GA

```
1 Population := RandomInitialization()
2   while True:
3       for each Solution in Population:
4           Evaluate Solution
5           Assign Fitness to Solution
6       newPopulation = SurviveAndBreed(Population)
7       Population = newPopulation
8   end while
```

Stopping Conditions This algorithm can run for a predetermined number of generations, indefinitely, or until another specific criterion is met. Consider the problem of finding a way of combining 4 operands with 3 operators to achieve a particular value. There are often many ways to solve this problem. If one was to use a GA to solve the equation, the algorithm could stop as soon as it had valid solution values for a, b, c, d, and the 3 operators which satisfied the equation. For example:

$$a \text{ op}_1 b \text{ op}_2 c \text{ op}_3 d = x$$

$$3 \times 7 \times 3 + 5 = 68$$

$$9 \times 7 + 8 - 3 = 68$$

Solution Encodings Now lets look specifically at what is meant by a solution. First, GAs usually have some encoding based ultimately on a string of 0s and 1s, called a bitstring¹. Continuing with our example, we know that there are 4 operands which

¹Other genetic alphabets are possible as well, though less common.

have a value between 0 and 9, or 10 values total. To encode that in a bitstring we use the values 0000-1010. We could also include some error correcting code to randomly reassign the bits if they go outside of the values, ensuring that any solution randomly generated contains valid data (we could also use more bits and/or arbitrarily assign values via modulo arithmetic, but this is the most instructive method for our current purposes). Next, we have the operators, which can be +, −, *, or /. These fit nicely within the 00-11 bit range, with no need of error correction. So we have a bitstring with the form xxxx-xx-xxxx-xx-xxxx-xx-xxxx², 22 bits which satisfy the constraints of our problem. The second line of the above example would be 0011-10-0111-10-0011-00-0101.

Fitness Functions Following along with the algorithm,

we need to assign fitness. In this case the closer one is to the solution, the better, usually ³. There is research showing that a fitness function should be differentiable, at least as far as the solution space. Point discontinuities aren't an issue if they occur outside of the solution space, which is important for us because we're going to make use of one. Specifically, the function

$$F(s) = \frac{1}{|E(s) - x|}$$

Where $E(s)$ is the result returned by evaluating s , the numeric string. So if we had the string $3-6*6+2$, then $E(s) = -16$. Assuming x is still 68, then the fitness for that particular s would be $\frac{68}{84} = 1.19E - 2$, extremely low. When $E(s) = x$ or $F(s) = \infty$ we break out of the infinite loop. This would be a discontinuity, but the function is still differentiable across where we're evaluating it.

²We use the hyphens here only for readability. The bitstrings contain only 1s and 0s.

³There are examples of x where this won't work as well; in a shortened version of our example problem, for instance, if the target is 25, $2 \times 3 \times 4$ will quickly dominate the fitness landscape but isn't actually any closer to a valid solution than $5 \times 5 + 9$.

Breeding and Survival Now that we have a fitness function, we can evaluate the entire population and determine who has the highest fitness. With a random seed, the first generation is usually not very fit. Regardless, the next step is to see who survives and who breeds into the next generation. Survival is usually an arbitrary matter of copying the best solution(s) *in toto* to the next generation.⁴ This is typically referred to as elitism, and it is usually a percentage around 10% of the population that is uncritically copied into the next generation. Properly done, this guarantees monotonically non-decreasing fitness of the best solution from one generation to the next.

The next step is to pick some fraction of the population as breeding stock. The most fit are generally given preferential treatment, but not exclusive preference. This is in large part because in GAs as in life, genetic diversity is a critical trait to the overall fitness of a population. For GAs, it means that diversity speeds convergence to ensure that even the less fit have a chance to propagate into the next generations. The method we employ, a fairly standard one, is Roulette Uniform Selection. To get an intuition for the algorithm, see 1.2. In it, you can see that RUS chooses markers (represented by the arrows) equally spaced between the beginning of the population and the end. Everywhere a marker falls means a copy of that solution gets passed into the breeding population for the next generation. This is usually guaranteed to get at least 1 copy of the most fit individual, but everything else is based on chance. There is some discussion that suggests that proportional selection provides the weakest selective pressure of several types of selection processes and thus that other methods should be employed or that supplementary approaches be taken(Back, 1994). While we have found this to be true to some extent selective pressure that is too strong can cause premature convergence(Affenzeller and Wagner, 2003), we implemented tournament selection, linear selection, and a Biased Random Key selection scheme (Ruiz et al., 2015) before settling on RUS because in testing the GA would typically

⁴Some variations have ages, where all solutions will live a certain amount of time, and more fit solutions have longer lifespans than less fit solutions. These will not be covered further in this document.

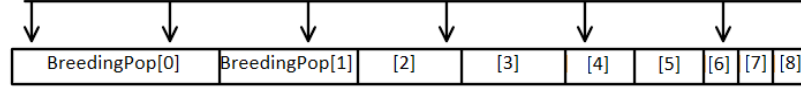


Figure 1.2: An example of RUS. The bar represents the cumulative fitness of the population. The arrows represent which members of the population go on to become a breeding member. In this example, 3 gets skipped even though it has higher fitness than 4 and 6, while 0 gets copied into the breeding population twice.

converge to minima prematurely. Thus we are actively choosing to preserve diversity over rapid but premature convergence.

With a breeding population in place, we can begin the breeding process. This is typically accomplished via an operation called crossover, which I will explain below.

<i>A</i>	<i>1001</i>	<i>10</i>	<i>0011</i>	<i>11</i>	<i>1001</i>	<i>00</i>	<i>0111</i>
B	0011	01	1000	01	0001	10	1001

We begin with two solutions. Crossover takes and returns 2 bitstrings. It also has several subtypes, which I will illustrate in sequence. First is one-point crossover. This means that before crossing, a crossover point is chosen and offspring are produced as a copy, and when this point is reached, the offspring cross over and begin taking material from the other parent.

<i>A'</i>	<i>1001</i>	<i>11</i>	1000	01	0001	10	1001
B'	0011	00	<i>0011</i>	<i>11</i>	<i>1001</i>	<i>00</i>	<i>0111</i>

Two point crossover is similar to one point, except that crossing happens twice.

<i>A'</i>	<i>1001</i>	<i>10</i>	0000	01	0001	10	1111
B'	0011	01	1011	<i>11</i>	<i>1001</i>	<i>00</i>	0001

Notice that here the final digit of *A'* and the second digit of *B'* become invalid (1111 is not between 0000 and 1001). This case is not controlled for in Crossover, but rather handled later by evaluating the offspring in the catch-all error function which is invoked before evaluation.

The final standard type is uniform crossover, which makes a check at each bit to crossover. It results in much more mixing, depending on the probability of a crossover event. One advantage is that it treats the beginning and end as the same, which can't be said for either of the first two. Another is that it allows the designer to specify, directly and exactly, how much gene mixing should occur on average.

One thing that might be noticed is that regardless of where the crossover point is, with these methods if both A and B contain a particular bit in the same location, it will appear in both offspring. This is one reason that diversity is important: if the population becomes too homogeneous, it will be unable to change except through random mutation, which we discuss shortly.

One other form of crossover we will deal with is one that counters this potential vulnerability. It is a shifted crossover, so that one bitstring shifts forward a random number of bits, and then crossover proceeds normally.

Other forms of crossover are possible, though they are not as widely represented in the literature. One is a modified uniform crossover that checks to cross only at each “word”, that is at each column representing a digit or operator in our example. This gives the designer some control over how much contiguous information is exchanged per crossover. Other variations with three or more parents, or even random asexual reproduction are possible. Logical operations are viable, though again care must be taken to not increase homogeneity overmuch.

Mutation Mutation is fairly straightforward. Usually after crossover and before insertion in the next generation, that is, only affecting the offspring of breeding and not elitism, each bit in the bitstring has a chance to change. The algorithm is perhaps the most instructive:

1.3: Mutation

```
1 for (Solution s in Crossover(A,B)):
```

```

2         for each bit in s.Bits:
3             if(MutationChance > Random(0,1)) bit = !bit
4         end for
5     end for

```

There are some implementations that vary in that they will change random values to 1 or 0 rather than flipping bits (in other words, values will change about half as often). A standard value for mutation is small, about $\frac{1.0}{\text{Solution.Length}}$ which means on average 1 bit will change per solution per generation.

What is less straightforward are the effects of mutation over a population. While values of 0 often stagnate in local minima, an upper correlate doesn't seem to exist. That is, one could set mutation high, say 25%, and turn off crossover entirely, and proceed with elitism and mutation alone and arrive at solutions. In practice, this is much slower than using crossover. A general rule of thumb is to keep mutation low, and increase it even more slowly to combat stagnation.

Drawbacks While GAs have great versatility, there are some drawbacks which significantly limit their utility.

Swiss-Army Chainsaw First, GAs are not the perfect solution for anything. At their core, they are a biased-walk⁵. This means that while they will come to a local optima, there is no guarantee they will achieve a global optimum. If there exists a tailored solution for a problem, using that will probably work faster and better.

And Quick to Anger Second, GAs are subtle things. The fitness function, not given its due in this writeup, can be the difference between a quickly converging

⁵With a random-walk on one side of the spectrum and a guided approach, such as gradient descent, on the other.

solution and processors spinning their wheels for days or months coming to one unsatisfactory solution after another. A GA will optimize the fitness function, and that's all it will do. So if you want to maximize a metric, say accuracy for a classifier, be aware that it might do exactly that by simply guessing the most prevalent answer in the dataset. This will get it to a local optima, and it might be surprisingly difficult to get it out of it.

Furthermore, there are hyperparameters which effect the GA directly but can be difficult to tease out. What should the elitism percent be? It probably depends on your other parameters. There are ways of optimizing these, and they themselves might be amenable to a further GA, except that evaluating them is time consuming; should your fitness function be speed of convergence? Or the best solution arrived at within 100 generations? That might seem too long, but use fewer generations and you run the risk of invoking too much sensitivity to starting conditions to draw meaningful conclusions. There are some rules of thumb to assist with these situations, but they only mitigate the problem, they don't eliminate it entirely.

Toolset Finally, a GA is only as good as its toolbox. On Earth, that toolkit was physics. All of physics, and massively, embarrassingly parallel at that. That's difficult to take advantage of digitally, where you not only have the responsibility of developing an encoding but also defining the universe your population lives in. For instance, the heart of this paper is whether to use a GA to optimize a classifier or to use a GA to classify things. The classifier has theory underpinning its toolkit, the GA has only whatever fitness function and encoding it is supplied. Or, to get back to our example, it might speed convergence to increase mutation rates and restrict crossover to occur only at the breakpoints of binary words. The downside of this is that GAs are supposed to be able to solve any problem, and while they can, they also require a certain amount of customization to not waste everyone's time. The harder the problem, the more customization that is usually required. And at that point, if a tailored solution of some kind exists it's probably easier to code up and implement

than an equivalent GA. At their core, the GA is a biased walk, but building in paths will hopefully make that walk much quicker.

Theoretic Underpinnings Intuition is often insufficient for or even anathema to scientific inquiry, and so far that is all we have relied upon to understand why GAs work. The Fundamental Theorem of Genetic Algorithms is used to explain much of it. First, where we explicitly represent populations as collections of bitstrings, we may impose an additional ordering on them, the schema. Returning to our example, consider the equations:

$$3 \times 7 \times 3 + 5 = 68$$

$$9 \times 7 + 8 - 3 = 68$$

$$9 \times 7 + 6 \times 2 = 75$$

These translate to the bitstrings

$$\mathbf{0011-10-0111-10} - 0011 - 00 - \mathbf{0101}$$

$$\mathbf{1001-10-0111-00} - 1000 - 01 - \mathbf{0011}$$

$$\mathbf{1001-10-0111-00} - 0110 - 10 - \mathbf{0010}$$

Let's just assume that our x is close to, but is not 68. Let's say it's 71. This means that each of these bitstrings will have a relatively high fitness. Specifically, the first two have a fitness of $\frac{1}{|71-68|} = \overline{.3}$ and the third has a fitness of .25. However, a close inspection of all bitstrings side-by-side shows that they have a considerable amount of overlap. All begin with odd numbers multiplied by seven, etc. You can see the overlapping sections in bold, but pay careful attention to the long contiguous sequence. Schemata are a way of considering a population theoretically. A schema introduces a third character into the alphabet of bitstrings: an * indicating either 1 or 0. Schemata are of any length, and may be defined by their offset and bitstring (their

length may be obtained from their bitstring). Thus, offset 0 and “***1-10-0111-**” is a valid schema which describes both solutions. In fact, there is one schema that describes both strings, which is already represented by retaining the symbols where it is bold and replacing it with * where they don’t match.

It should be obvious that doing any calculations with schemata are infeasible, simply because for even short bitstrings, the possible schemata to describe the population increase exponentially. Let m be the length of a bitstring, and S be the set of schemata which can describe the population. Then let

$$|S| = \sum_{i=1}^m 3^i(m - i + 1) = \frac{3}{4}(-2m + 3^{m+1} - 3)$$

While we could try to constrain this by only using the schemata that describe the currently existing population, that problem is also exponential, and potentially worse computationally, because any member of the population has

$$\sum_{i=1}^m 3(m - i + 1) = \frac{3}{2}m(m + 1)$$

schemata that describe it, but then these would need to be compared with the sets generated by all 2^n combinations of members of the population.

However, feasibility of computation aside, we can use this to gain a further and more formal understanding of how GAs function.

Informally, if we assume that schemata describe our population, whatever they may be specifically, we may also assume that short, more fit schemata will have a greater than average fitness than is represented in the population, and as such these short, fit schemata are likely to increase in representation throughout the population. Shorter schemata will survive because longer schemata are more likely to be broken up by crossover. Three more concepts need to be understood before the equation itself: First, is the order of a schema H , which is the number of non-wildcard bits it contains. Higher is more specific. Second is the defining length, which is the distance between

the first and last non-wildcard bits. If we return to our example, and let $H_a = \text{offset } 0, \text{ “***1-10-0111”}$ and $H_b = \text{offset } 0, \text{ “*0*1-10-**11”}$, then $o(H_a) = \delta(H_a) = 7$, while $o(H_b) = 6$ and $\delta(H_b) = 8$. Third is $f(H)$, which describes the average fitness of a schema. This is defined as

$$f(H) = \sum_{s \in H(P)} \frac{F(s)}{|H(P)|}$$

where $H(P)$ is the schema H applied to the population P , which returns a subpopulation of solutions, and where s is one such solution returned.

With these concepts understood, the Fundamental Theorem of Genetic Algorithms is as follows:

$$r(H, t+1) \geq r(H, t) \frac{f(H)}{\bar{F}_t} \left[1 - \left(p_c + o(H)p_m \right) \right] \quad (1.1)$$

Where \bar{F}_t is the average fitness of the population at time t . p_c and p_m are probabilities of crossover and mutation, respectively, and $r(H, t)$ is the number of representations of a schemata H at a time step t in a population. The type of crossover plays a role, here. Depending on implementation, in single point crossover the probability of crossover occurring is usually ⁶. Instead, a random number from 1 to L is usually chosen, with each index being equally likely, and crossover occurs at that index. Thus, for single point crossover,

$$p_c^{SinglePoint} = \frac{\delta(H)}{L-1}$$

For two point crossover, the odds of breaking a given schema is much more likely, because it is the outcome of 2 events not happening, that is

$$p_c^{TwoPoint} = 1 - \frac{L - \delta(H)}{L-1} \frac{L - \delta(H)}{L-2}$$

⁶Often, at any rate. When it isn't, it can be used as a sort of ersatz elitism, simply passing copies of both parents into the next generation. However, if employing a significant level of elitism, there's a good chance at least one parent is already in the population, and doing this would create a duplicate, which is a waste of a slot in the population.

from which we get the general

$$p_c^{NPoint} = 1 - \frac{(L - \delta(H))^n}{\frac{(L-1)!}{(L-1-n)!}}$$

for n point crossover.

Uniform crossover is implemented differently, and is generally done with a rate, which we'll call γ . Since this is the case, it makes calculating p_c more straightforward.

$$p_c^{Uniform} = 1 - \gamma^{o(H)}$$

So, while representations for schema which are more fit than others will increase over time, the particular type of crossover can have a significant impact on how much representation they gain. It is worth noting that a uniform crossover with even a moderate rate of crossover (say, .3) can rapidly lead to the eradication of all higher-order schemata. Also worth noting is that when a schema applies to both solutions, both offspring will also belong to that schema using standard crossover methods. Finally, if an implementation includes a probability other than 1 for any of the forms of n point crossover, that probability is simply multiplied to the appropriate p_c .

A few observations about this function. As overall length of the bitstring increases, the inhibition of single-point crossover decreases, but inhibition of n point crossover generally increase, and if the mutation rate is linked inversely to length then it does as well. Uniform crossover is less directly linked to length, though not independent: as L increases, the numbers of higher order schemata increase exponentially. Survival of a particular schema becomes very unlikely without a strong selective pressure toward retention. Further, high order and fitness schemata with greater defining lengths rapidly become unlikely to obtain except through elitism.

Motivations Over the course of researching how GAs were being used in recent times a broad pattern emerged. With regards to classification, there were two basic schools of thought: one in which GAs were used to optimize classifiers and one which used GAs as classifiers directly. Both camps have *prima facie* impressive examples of these approaches. Thus, this project was born: to attempt to answer which approach is more generally applicable.

GA are widely used for numerous purposes, but we seek to ascertain their suitability for pattern recognition, specifically classification. In this paper, we attempt to determine how suitable GAs are for the task of classification. To determine credibility, we propose 3 tests. First, we will run a GA on the datasets acting directly as a classifier. Second, we will run two classifiers, a lone Decision Tree, and a Naive Bayes classifier with default settings as a control. Finally, we will run the same classifiers optimized through a GA which will run for a modest number of generations. We will collect confusion matrices from the resulting classifiers and compare them.

To ensure that our approach is generally applicable, we propose datasets from divergent fields of study and with data in different configurations. With minimal adjustments, the program we have written is capable of automating this process over almost any dataset, but we have chosen 3 from the UCI repository(Lichman, 2013) : Yeast Dataset (Yeast)(Paul Horton, 1996), Bach’s Chorales Dataset (Bach)(Daniele P. Radicioni and Roberto Esposito, 2014), and Cardiotocography Dataset (Cardio)(J. P. Marques de S et al., 2010). This gives us 4 different configurations to use, as Cardio has two modes that it runs in, with the pattern class code (1-10) or the fetal class code (Normal, Suspect, Pathologic), which we refer to as Cardio and CardioNSP, respectively. This gives us data from biology, music, and medicine, which serves as a broad start. However, we are also making the code available in its entirety for anyone who wants to extend this to other domains of study.

Priors Going into this project, a case for either side could be made. On the case for the Pure GA approach you have a few points. First and foremost, versatility: the GA is only limited by the encoding, and a clever encoding could exploit nuances that people wouldn't be likely to notice in the data. Secondly, there's something about the simplicity of only having 1 component to debug: this could speed development which would mean more effort could be spent developing the encoding and the fitness function. One con is the inverse of the first pro, that encoding needs to exploit the nature of the data, and so much time can be spent customizing the approach to the data, but this is also antithetical to the idea of a generic solution to classification, so whatever encoding we use must be good enough to apply to many problems.

For the Hybrid camp, the pros are primarily that the GA gets to leverage the theoretical robustness of the external classifier. That is to say that there has been a great deal of work to make classifiers extremely good at what they do and writing a GA to compete with or exceed beyond that work is difficult. There are several cons, though; the external classifier needs to be written and debugged separately and then in conjunction. Also, there are now 2 or more entities to be maintained which means much less time can be spent on any one project, unless you simply tie into some other classification package, though that may have its own challenges.

Thus, before going into this project, we slightly favored the hybrid approach. But we wanted to make sure that there was plenty of versatility for the GA to make use of, so for the implementation of our pure GA we settled on CellNet ([Kharmah et al., 2004](#)), which is a variable length GA which has a new breeding operator. We discuss this project in depth in Chapter 2.

Literature Review

Hybrid Approach In [Schuman et al. \(2014\)](#) they use classifiers to breed numerous neural networks in parallel and test them against MNIST. In [Ocak \(2013\)](#) the authors use a support vector machine (SVM) optimized by a GA to predict fetal

well-being, with considerable success. In [Marchetti et al. \(2013\)](#) GAs were used for feature selection and then the features generated were passed to a logistic regression classifier. In [Wu et al. \(2015\)](#) GAs were used in conjunction with particle swarms to optimize a neural network for predicting rainfall. While GAs performed better in conjunction with the particle swarms than alone, the idea of using a GA to build a better classifier is present. [Chou et al. \(2014\)](#) and [Duan et al. \(2014\)](#) discuss using a GA to optimize another SVM, this time emphasizing the mileage obtained from leveraging the SVM for curve fitting while the GA handles the optimization of the SVM itself. [Devos et al. \(2014\)](#) takes a similar approach, but instead focuses on using the GA to determine which combination of preprocessing methods to use. The GA is also used to determine two meta parameters for the SVM itself. Once these are determined, the SVM is used to handle the classification. In [Uysal and Gunal \(2014\)](#) they use GAs to focus their Latent Semantic Indexing approach on promising semantic features. They use two different approaches and find that both are much more effective on a wide range of tests than the approach without the GA optimization. [Salari et al. \(2014\)](#) used an ensemble approach which is quite novel. First, they use doctors to decide which features of the datasets in question to use. Then, they give these features to a Feed Forward Neural Net(FFNN) on one hand and a GA on the other. The GA generates several different arrays of features, and then these arrays and the results from the FFNN are fed to a k nearest neighbor to find fuzzy classes, then those classes are iteratively pared down until they are no longer fuzzy. They apply their model to multiple datasets, and compare across a wide variety of methods with a variety of metrics, over which they show statistically significant gains on nearly every method, metric, and dataset. [Alexandre et al. \(2015\)](#) hybridizes a GA with an Extreme Learning Machine, with considerable gains in both binary and multiple class classification over several learning methods.

Purist Here, we look at papers where GAs act directly as the classifier. We have included papers where rules for classification are generated. [Dehuri et al. \(2008\)](#)

uses two different GA approaches to classification rule generation, one a simple one similar to the “canonical” approach and one a multi-objective optimizer. The multi-objective GA performed well, though areas for improvement were discussed in the conclusion. One area particularly limiting the GA was the number of attributes the GA was working with. The interestingness of the discovered rules was quite high, though sometimes the comprehensibility was lacking. Still, the rules were highly predictive on the datasets employed. In [Kozeny \(2015\)](#) they used 3 GAs to calculate credit scores, and compared their accuracies. While they achieved interesting results with their methods, the most promising one scales at $O(2^L)$, which makes it unfeasible for computation except on short feature sets. In [Srikanth et al. \(1995\)](#) variable length GAs are used to draw fuzzy ellipses in a decision space, and thresholding is used to make the borders crisp. This approach is shown to be comparable over their selected dataset to a back-propagation neural net (BPNN).

[Fidelis et al. \(2000\)](#) uses a GA to develop rules for diagnosing breast cancer and dermatology. They achieve 95% accuracy on the dermatology but only 67% on the breast cancer, which is, by the author’s own admission, a much more difficult dataset with a great deal more noise. Beside the results, the rules themselves were of interest, and evolved 3 separate times from different random seeds. The rules developed seemed to hit the knowledge discovery trifecta of predictiveness, comprehensibility, and interestingness.

In [Hoque et al. \(2012\)](#) and [Li et al. \(2012\)](#), GAs are used to solve an intrusion detection problem. While both papers boasts a discovery rate of nearly 100%, if one ignores the denial of service attacks their discovery plummets. Unfortunately, it isn’t clear that the authors are entirely at fault for this; the data which might have been used⁷ for the DARPA challenge contained 5,283 non-DoS attacks, but 391,000 DoS attacks (it also contained 97,000 non-attacks). Its small wonder that the GAs would optimize according to capture the most numerous classes in the data. [Tseng et al. \(2008\)](#) is another example of rule discovery, but this time applied to land-cover

⁷The authors don’t elaborate and there are several versions of the KDDCup data.

classification. They specifically use a GA as an alternative to other methods such as a Neural Net(NN) or other Bayesian classifiers because the GA has shown that the rules it discovers are more comprehensible, even if less predictive. In other words, while NNs may be good at solving a problem, exactly how they solve it is not always clear, and that can be problematic for many domains. Unfortunately, while they get good accuracy they don't do a head-to-head comparison. One possible reason is because the database is very small, at only about 400 samples.

Finally, we will discuss the CellNet family of papers which inspired one prong of our approach in much more detail in Chapter 2. In the original CellNET paper ([Kharm et al., 2004](#)), they used a variable length GA to classify the [CEDAR \(2002\)](#) database. While they obtained modest results, the stated goal of CellNet was to develop a GA which could approach any dataset with minimal intervention. They continued in [Kowaliw et al. \(2004\)](#), where they employed two populations of competitive solutions called hunters and prey, where hunters are trying to classify a handwritten digit from the CEDAR database and prey are trying to obscure said image. The results in this paper were much more impressive, and their overfitting problem diminished significantly as well.

Chapter 2

Methods and Implementations

2.1 Overview

In this chapter we'll discuss the design decisions we've made in detail. We have 3 distinct phases. The first phase, preprocessing, is converting the data files into a unified dataset in memory and configuring for the following phases. The second phase is the hybrid approach where we optimize external classifiers, followed by the purist approach where we use our genetic algorithm (GA) to develop classification rules. Each of these approaches generate confusion matrices which we analyze.

The general flow of the algorithm can be seen in [2.1](#). Loading and normalization gets all algorithms on the same page, ensuring an apples-to-apples comparison. First we have the hybrid approaches. Within a hybrid approach, we first see what optimizing without including features yields; this is referred to in the code and in the program as the baseline approach. It has all the same constraints as the parent approach. After the baseline, we optimize a second time, this time including feature selection, by which we mean that we characterize a dataset with n variables as either included (1) or excluded (0) in a bitstring, and encode the same variables to the classifier as in the baseline method. We have selected two distinct classifiers: a multiclass naïve Bayes algorithm and a simple single decision tree. Each of these are run twice per

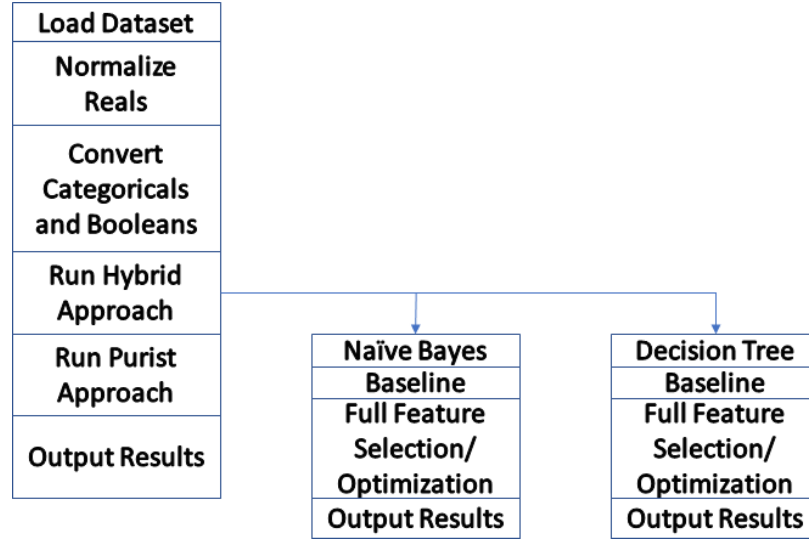


Figure 2.1: Birds-eye view of the flow of the program. Hybrid approaches are not run in parallel, because at time of coding MATLAB doesn't support multi-threading via a COM server.

dataset, once with feature selection disabled (the baseline) and once with it enabled.

We will discuss those methods in more detail in their respective sections.

The purist approach is much more straightforward. There is only one mode which it runs in, there's no explicit feature selection. That is, there is feature selection, but all features are available to the algorithm at any time, though some may not be included. This portion of the algorithm is threaded.

2.2 Preprocessing

We do some preprocessing of the data. First and foremost, there is a text file that is read which describes the dataset and points to where it is on the filesystem. Below is an example which tells the program where it can find X and Y and how to parse them.

2.2: Cardio Config File

```
1 #Dataset Name
2 CardioData
3 #Class Names File
4 ../../Data/Cardio/classNames.txt
5 #TrainingSet X Path
6 ../../Data/Cardio/trainingXY.csv
7 #TrainingSet Y Path
8 ../../Data/Cardio/trainingXY.csv
9 #TestingSet X Path
10 ../../Data/Cardio/testingXY.csv
11 #TestingSet Y Path
12 ../../Data/Cardio/testingXY.csv
13 #X ignore list, comma separated and starting with w if it's a whitelist
14 (otherwise, blacklist)
15 b, 29, 30
16 #Y ignore list, as above
17 w, 29
18 #Categorical Variables, white/blacklist, comma separated
19 w,
20 #Boolean Variables, as above
21 w,
```

For instance, in this case X(the data) and Y(the labels) are in the same file, but represented as different columns. They could easily be stored as two files. After those files are explained, the next uncommented line describes the columns to ignore or include, specified with b for blacklist or w for whitelist respectively. In this example, columns 29 and 30 are ignored for X, but only 29 is included for Y. This is because for this dataset, there are two sets of labels and thus two separate description files to use the file differently. Using the same notation, we can declare categorical and

boolean variables for X. Y is assumed to be categorical.

After we read how to parse the file, we read the files themselves. At this point we also convert booleans and categorical variables to doubles so that they can fit in the same matrix. First, however, we want to normalize the Reals. First we gather max, min and mean from each column in the dataset. Then we use a function to squeeze the values down between .1 (b) and .9 (t) for reasons that will be seen later in the section on the purist approach.

$$x'_i = b + (t - b) \frac{(x^i - x_i^{min})}{x_i^{max} - x_i^{min}}$$

Next, categorical variables are given the treatment motivated and described fully in [Zhang et al. \(2015\)](#), the conclusion being that every category label is replaced with a real number which maximizes Pearson's Correlation Coefficient. That is,

$$\begin{aligned} X &= X_{\mathbb{R}} \cup X_{cat} \cup X_{bool} \\ X_{\mathbb{R}} &= \{\mathbf{x}_1, \mathbf{x}_2, \dots \mathbf{x}_n\} \\ X_{cat} &= \{\mathbf{x}_{n+1}, \mathbf{x}_{n+2}, \dots \mathbf{x}_c\} \\ X_{bool} &= \{\mathbf{x}_{c+1}, \mathbf{x}_{c+2}, \dots \mathbf{x}_b\} \\ 1 &\leq i \leq c - n \\ L &= \{x_i | \mathbf{x}_i \in X_{cat}\} \\ C_{\ell} &= \{\mathbf{x}, i | \mathbf{x} \in X \wedge \mathbf{x}_{n+i} = \ell \in L\} \end{aligned}$$

Where X is the dataset, $X_{\mathbb{R}}$ is the real portion of the dataset, and X_{cat} and X_{bool} are the categorical and boolean portions. The index i iterates over the columns of X_{cat} , which lets us derive L, which is the set of all categories in the dataset. L in turn gives us a means of devising C_{ℓ} , that is, the subset of X which consists of all members of x which belong to the category ℓ . Now it is possible to look at C_{ℓ} and determine which

values will maximize r^2 for each label ℓ , which we here call $R(\ell)$.

$$R(\ell) = \frac{\sum_{\mathbf{x} \in C_\ell} \sum_{j=1}^n x_j}{|C_\ell|n} \quad (2.1)$$

It can be seen as the mean of all the other values over C_ℓ . Calculating this in practice is much more straightforward: simply step through X one sample at a time, and maintain running sums and counts for each unique label, calculate the means at the end and then extend $X_{\mathbb{R}}$ with the newly calculated values. In the case of multiple categorical columns, unless there is a perfect correlation between two category labels each label will have its own value (though this can't be proven to be unique, only generated from a unique set of numbers).

Booleans are only given the treatment of being converted to values .25 for false and .75 for true. Again, the reasons we don't use 0 and 1.0 will be made clear in the section on our purist approach.

Now that the data has been modified, some additional bookkeeping is accomplished. Conversions to numerics from string class labels and vice versa are computed and stored, since mathematical approaches prefer integers while human-readable outputs are in the terms given us by the dataset. Also, global values such as Elitism Percentage and Population Size are modified at this point and are effectively constant for the rest of the program. Variables that may be configured by the user are: Max Generations, Record Interval, Population Size, and Complexity bounds. The Max Generations sets the stopping condition of the algorithms, and defaults to 100. The Record Interval determines how often to save data to the disk. Data is collected every generation, but is only saved to disk in where $G \bmod (I) = 0$, and the default value of I is 25. Complexity bounds are discussed in more detail in the purist approach, and have no effect on the hybrid approach. Other modifications to semi-constants are made at this point determining the length of chromosomes for both approaches based on the characteristics of the datasets, particularly the number of features and number of classes.

2.3 Hybrid Approach

As mentioned previously, the hybrid approach consists of 2 methods which each consist of two different ways of running them. First we will discuss the multi-class naïve Bayes (McNB) approach, followed by the decision tree (DTree) approach.

McNB Naïve Bayes is one of the most basic of classifiers, but it is powerful and versatile. Without going into extreme detail, it generates probability distributions for each class across every dimension in the feature set from the training data, and picks the most likely class for a given sample point. Typically, the probability distributions are Gaussian, however any density function can be used. We use this because it should provide a fairly low bar to compete against; support vector machines (SVMs) are much more complex, tend to be extremely reliable and robust, and are close to something resembling the industry standard, but don't perform well with multiple classes. McNB is closer to statistical modeling and is not what we consider machine learning, though no bright line distinction exists. It is a theoretically grounded but simple statistical method well suited to being a first pass at the data or being used in conjunction with other methods. Being simple, it is also relatively fast- only 2 passes through the data are necessary to build the parameters for the PDFs, so building the model can be done in linear time. Once built, checking a given variable can be done in constant time.

$$P(A|B) = \frac{P(B|A) * P(A)}{P(B)} \quad (2.2)$$

While that is the standard formulation of Bayes' theorem, in our case it is more useful to reframe it thus¹:

$$P(\omega_j|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_j)P(\omega_j)}{p(\mathbf{x})} \quad (2.3)$$

Here, $P(\omega_j|x)$ is the likelihood of x belonging to a particular class. Upper case P s are simple probabilities, lower case p s are more complex functions. So $p(x|\omega_j)$ is the PDF,

¹Thanks to Dr. Hairong Qi for teaching this formulation.

and $P(\omega_j)$ is the prior, which can be thought of as *a priori* how likely a particular class is to present. To build the PDF, if we're using a Gaussian, we need mean and standard deviation for each class. The Gaussian PDF is built using the training set, tested on the testing set, and the results are scored in a confusion matrix. This can be determined from the dataset, in which case it uses the frequency in the Training set to generate priors, or set manually. In either case, this can be seen to scale a particular PDF. In fact, this is similar to what $p(\mathbf{x})$ does except that where $P(\omega_j)$ scales a class, $p(\mathbf{x})$ scales all classes, and it serves as a normalizing factor to constrain values between 0 and 1. It could be established using the law of total probability, or it could be some arbitrarily high constant². Thus, the specifics of $p(\mathbf{x})$ are largely irrelevant for our purposes. Rather, we will focus on the parameters to the MATLAB classifier we invoke.

Our implementation, which we'll refer to as the McNB optimizer³ optimizes the `fitcnb`⁴ function in MATLAB over the following parameters: distribution, kernel, score transform, and priors. Further, it optimizes over the dataset by choosing which features are included. It is entirely defined by its bitstring, the first several bits correspond one-to-one to the features in the dataset. An optimizer with all 1s (or all 0s to avoid having no data) will include the entire dataset. Otherwise, a 1 indicates that the column is included, a 0 removed.

The distribution uses 2 bits and can be any of the following values:

- Kernel uses a smoothing function, described below.
- Multinomial represents every class as a single multinomial distribution.

²It doesn't really make a difference, since the selected class will just be the one with the highest score given \mathbf{x} . Furthermore, if it affects all classes equally nothing is served by making complex calculations every time the classifier is called. Simply calculate the highest value it could take initially and use that in subsequent calls.

³To avoid confusion, our optimizers are optimizing classifiers, they are not classifiers but optimizers. Later, we present our classifier.

⁴For much further detail on Mathworks' implementation see <http://www.mathworks.com/help/stats/fitcnb.html>.

- Multivariate multinomial characterizes each feature as an independent multinomial distribution based on the unique values found in the feature.
- Normal distributions behave as described above.

Kernel type uses two bits, though these go unused unless the distribution is kernel. Then the variables are smoothed via various functions outlined below.

- **Box** uses a uniform, box-like smoothing window.
- **Epanechnikov** is a very efficient, rounded kernel. Minimizes Asymptotic Mean Integrated Square Error (AMISE)([Stefanie Scheid, 2004](#)) therefore optimal in that sense.
- **Gaussian** is a standard normal function but used in this case for smoothing.
- **Triangular** is another form of smoothing, with a peak of 1 at 0 and zero at -1 and 1.

Regardless of which form of smoothing, the goal is the same: to create a distribution of a random variable which can then be modeled. This is done using something like a histogram, which is then smoothed into a continuous function using the kernel chosen above. This becomes $p(x|\omega_j)$ in the equation [2.3](#).

For priors, each class extends our optimizer's bit length by 3 bits. Each class then has a prior in the range $1 + [0, 8] = [1, 9]$ which is later summed and turned into a probability distribution summing to unity. For instance, if a database has 2 classes, and an optimizer has assigned one a prior of 3 and the other a prior of 7, these are converted into percentages of 30% and 70%, respectively. These become the $P(\omega_j)$ in equation [2.3](#).

Finally, the score transform takes up 3 bits and can be any of eight values. This is used internally in the MATLAB function. It can take on any of the following values:

- DoubleLogit transforms the score to $\frac{1}{1+e^{-2x}}$

- Invlogit $\log(\frac{x}{1-x})$
- Logit $\frac{1}{1+e^{-x}}$
- None x
- Sign $\frac{x}{|x|}$, or 0 when $x = 0$.
- Symmetric $2x - 1$
- Symmetricismax 1 if max of class, 0 otherwise
- Symmetriclogit $\frac{2}{1+e^{-x}} - 1$

Once these are determined, the optimizer is evaluated. This means that the training set is passed to the optimizer, it is trained, and then the testing set is passed to it, from which we get the fitness of the classifier. Fitness is average accuracy. That is, suppose we have a confusion matrix C

C=	True:	ω_1	ω_2	ω_3	Total
	Predicted ω_1	4	6	5	15
	Predicted ω_2	2	2	9	13
	Predicted ω_3	8	2	110	120
	Total	14	10	124	148

The dataset in this case has 3 classes, ω_1 , ω_2 , and ω_3 , and has 148 total samples. Of those, 14 are class ω_1 , 10 are class ω_2 , and 124 are class ω_3 . Meanwhile, the classifier predicted that 15 of the samples were ω_1 , 13 were ω_2 , and 120 were ω_3 . To determine accuracy, the equation is $\frac{\sum_{i=1}^3 C_{ii}}{148}$. This is a good metric for relatively evenly distributed classes. However, in highly skewed cases as this one, this treats more rare classes as less important. For instance, in this case, the accuracy is $\frac{116}{148} = 0.784$, which might seem like it is doing a decent job, and maybe it is, if the concern is finding Cs. Average accuracy is slightly more complicated to calculate, but still straightforward

enough. First, let's define the Total column more formally:

$$T(\omega_i) = \sum_{j=1}^N C_{ij}$$

Where N is the number of classes. Thus, average accuracy, \bar{A} can be defined as

$$\bar{A} = \frac{\sum_{i=1}^N \frac{C_{ii}}{T(\omega_i)}}{N}$$

In our example, \bar{A} is .467, which seems more like the classifier is doing barely better than chance. In fact, if it had just guessed everything was ω_3 , accuracy would be higher (.833), but \bar{A} would have been .333. Further, \bar{A} is equivalent to accuracy if all classes are equally distributed, thus there is no disadvantage to using it. Average accuracy is a major factor to the fitness functions used in this project.

We will next discuss another type of optimizer, and then we will discuss what they have in common.

CTree Decision Trees are an algorithm which take a dataset and make usually boolean decisions from its features, which generates a hierarchy resembling a tree. They are very easy to compute, but usually aren't the most robust of classifier unless used in ensembles. However, finding an optimum decision tree has been shown to be NP complete (Hyafil and Rivest, 1976), so greedy approaches are often used to approximate the perfect tree. Decision trees are referred to as Classifier Trees or Regression Trees, depending on their task.

Decision trees are typically generated using a greedy algorithm to maximize the split criterion at each of several splits. The Gini impurity is $1 - \sum_i p^2(i)$, where $p(i)$ is the fraction of samples belonging to ω_i which reach the node. It is distinct from the Bayesian prior because it doesn't apply equally to all samples. For instance, there might be 10 classes in a dataset, but if only one class would reach a node, then the sum of $p(i)$ would equal 1, and the Gini impurity would be 0. Thus, it can also be

seen as the probability of *misclassifying* a sample based on the distribution at that node. Gini impurity is maximized at every decision, insuring that nodes are diverse. Gini impurity is closely related to entropy, and some decision trees are implemented using information gain instead; the difference in output is minimal, while Gini is marginally easier to compute. For completeness, entropy of a node may be defined as $E = -\sum_i p(i) \log(p(i))$ and it is possible to use entropy gain as the split criterion. A third criterion is twoing, which is quite different. It tries to find a division of samples whose class makeups are as homogeneous as possible and also make close to 50% of the samples at the node the node, and then it tries to find a split to make that grouping possible. For instance, if 4 classes were at a node, and two of the classes made up 50% of the samples at the node, the algorithm would try to find a split that would maximally separate those two classes from the others. To ensure meaningful decisions, there is usually some cap on the depth of the tree.

The next optimizer we'll discuss is the Classifier Tree (CTree) optimizer. This is optimizing MATLAB's `fitctree`⁵ function over the following fields: Merge Leaves, Maximum Splits, Min Leaf Size and Split Criterion. Each CTree optimizer is completely defined by their bitstring, which are typically much shorter than for McNB. It too begins with a representation of the features in the dataset, 1s for included, 0s for excluded, and either all 1s or zeros mean the entire dataset is included.

- **Merge Leaves** takes 1 bit and is either on or off. Merge leaves looks at leaves from a parent node and if the amount of their risk (a term which we believe corresponds to Gini impurity, but we can't find sources backing that up) and that of their offspring is at or greater than that of a parent. In our CTree optimizers, this takes up one bit of the bitstring.
- **Maximum Splits** defines how many splits a tree can have. The tree is built iteratively, layer by layer, splitting as needed until it hits this number. In our optimizers, 6 bits are reserved for it, yielding values of 3-66.

⁵See <https://www.mathworks.com/help/stats/fitctree.html> for examples and further details.

- **Min Leaf Size** This is the minimum number of samples that need to reach this node to be considered a standalone leaf. Beyond this number (specifically, at twice this number) a leaf become a parent node split into two children. Five bits are reserved for it, yielding values between 1 and 32.
- **Split Criterion** can take on 3 values. Gini’s diversity index as discussed above, twoing, and deviance. When deviance is selected, the rule is maximally reducing deviance with every split (effectively using entropy rather than impurity). With Twoing, it will try to make an optimally balanced tree, erring toward balance rather than composition (in practice, these tend to be similar to entropy based trees). These take up 2 bits of the CTree optimizer’s bitstring.

Optimizers Our optimizers use inheritance to share common code. So both CTree and McNB use many of the same mechanisms when it comes to evaluation and evolution. First, both of them use MATLAB as their engine. Unfortunately, while support is planned for a future release, evaluations done through the COM server (as opposed to done through the MATLAB SDK and compiler) do not support multi-threading, so even if multiple threads were used in the native code, there would be no performance gains to speak of. In fact, while we don’t have metrics any longer, execution was considerably slower when we were using the multi-threaded model. We did at one point make use of the MATLAB SDK to compile the MATLAB code into native, and this was indeed faster, but there’s considerable overhead involved and unless you have a MATLAB educational license, considerable cost. Thus we have opted for the sub-optimal but considerably more cost effective implementation.

There are many commonalities. For instance, initialization of a new Optimizer is really only dependent on the length of that class. The core mechanism is the same in both of these classes (and several others that we have implemented outside the scope of this thesis). Also, once an Optimizer is initialized, there may be errors. While the concrete classes can handle the details, in the abstract the general principle holds that once an Optimizer is initialized, it needs to be prepared for evaluation. For

instance, if CTree's split criterion is 3, when only 0-2 are allowed, then those bits need to be rerolled. The rerolling itself is common Optimizer code as are several utility functions, such as logical operators between two Optimizers.

Scoring binary or multi-class Optimizers, saving them, much of the file IO, most of the life-cycle of an Optimizer, and memory management is handled in the common Optimizer code, meaning that implementing a new type of Optimizer can take a tiny fraction of the time implementing a new optimizer can and even the MATLAB dependence is optional. The relevant code is actually in the Globals file and the Eval functions in the concrete subclasses. Optimizer does provide a virtual convenience method of ComEvalFunc which handles common cases, but there's no requirement for that to be called in a subclass. The upshot is that this could be used with an entirely different sort of function which wouldn't necessarily need to be a classifier at all⁶. It could easily be sub-classed and modified to optimize different criteria altogether. The other heavy lifter, in terms of inheritance, is done by Evolver.

Evolver Evolver is the class which makes up the bulk of the evolutionary algorithm. Where Optimizer provides a framework for the finer details, Evolver handles the broad strokes of evolution. It maintains a population of Optimizers and handles their life cycles in a way that is both extensible and straightforward.

This is in large part due to the fact that the evolution is entirely class-independent, implemented using templates. While it requires that the class being optimized is a subclass of Optimizer, that's really the only requirement; simply sub-classing Evolver and adding a new interface would allow dramatic changes to the function being optimized.

First, let's look at our modified algorithm, as this will provide more details.

2.3: Evolver Algorithm

```
1 AdvanceGeneration():
```

⁶We plan on using this framework to experiment with integer Linear Programming in the future, for instance.

```

2      //P is the population and a class variable
3      EvaluateAllOptimizers(P)
4      GetMetrics()
5      P.ReverseSort()
6      P = GenerateNextGeneration(P)
7      RemoveDuplicates(P)
8
9  GenerateNextGeneration(P):
10     BreedingPop := StochasticRUS(P)
11     NextGen := Elitism(P)
12     FillListFromBreedingPop(NextGen, BreedingPop, P.Count, UniformXOver)
13     MutateNonElites(NextGen)
14     return NextGen
15
16 FillListFromBreedingPop(N, B, size, Func):
17     E := B.Count * ElitePercent
18     while(N.Count < size):
19         k := j := RNG.Next(0, E)
20         while(j==k)
21             k = RNG.Next(0, B.Count)
22         for each offspring in Func(B[j], B[k])
23             N.Add(offspring)
24
25     while (N.Count > size)
26         N.pop()

```

So lets examine the high-points of these algorithms. While EvaluateAllOptimizers might seem straightforward, in the details of that function we can either use multi-threading or not (we do not if we are using the COM interface to MATLAB), and we maintain a hash table of all tested Optimizers and their fitness, along with secondary

characteristics if those are important. This is from an earlier instantiation of our system where evaluation was extremely costly and so the extra overhead was worth it to save cycles. This is only possible because performance is entirely defined by the bitstring, this lets us test each string once and never test it again. Finally, in `FillListFromBreedingPop`, `Func` is `UniformCrossover`, but that's just one of several modules supplied. In fact, as the signature is written⁷, it could easily take any sort of two-parent breeding function, with any number of offspring. Three or more parents could also be implemented if that was desired, though this would require minimal sub-classing.

`RemoveDuplicates` is also important, because any `Optimizers` that are removed are replaced with randomly generated new ones whose bitstrings are checked to be unique before replacement is finished, so the population size is maintained. The reason this is important is because the breeding selection we're using in `FillListFromBreedingPop` is a variation of the Biased Random Key model ([Ruiz et al., 2015](#)) which provides great selective pressure but makes duplicates more likely as the elites become more homogeneous. It is a modification because the model in the paper guarantees that every offspring will have at least 1 elite parent. Our implementation doesn't, because we're drawing both parents from the breeding population and because of RUS there's no guarantee that any `Optimizer` other than the one at `B[0]` will be elite. Instead, they are very likely to be elite.

The metrics we capture in `GetMetrics` are simply best and average fitness, but this provides an entry point to capture population metrics in a subclass or modification of the code. In `GenerateNextGeneration`, we use RUS and Elitism as discussed in Chapter 1. We also mutate the non-elites after our next generation has been determined.

⁷The signature is `Optimizer[] BreedingFunction(Optimizer A, Optimizer B)`- however, there is also a related function template provided which takes a variable number of parents.

OptimizerProgram There’s only one more major component to the hybrid approach, and that is the `OptimizerProgram` class, which handles hyperparameters to `Evolver`. How often to write data to disk, whether or not to multi-thread, population size, how many generations to run and file IO, as well as insuring all the directories for file IO exist are among the duties handled in this class. Incidentally, we employ what we refer to as a baseline mode, which means running `Evolver` two different ways. The baseline method runs `Evolver` with all columns turned on; in other words, it restricts the evolutionary process from functioning as a feature selector and only optimizes parameters to the classifier itself. Then it runs again, this time without the restriction. This provides a baseline comparison to see how much performance changed when feature selection is included in the optimization. There are of course many, many more details in the code itself, which is available in the appendix, and comments provide motivation for much of the detail in situ. This writeup should cover the high points, however, and give a reader an idea of what they are looking at in the code.

2.4 Purist Approach

In this section, we will discuss the implementation of a pure approach to classification. Classification is executed by the evolutionary algorithm itself. To understand all the parts working together, a bottom-up approach is instructive. However, to guide that discussion, let us begin by motivating the algorithm. For an evolutionary algorithm, we need a population of solutions to evolve. In this case, we borrow the terminology and much of the methodology from [Kharma et al. \(2004\)](#) and say the population comprises Hunters, which are the form our solution will take. While this paper may not be a perfect reimplementaion of theirs, it is strongly inspired. These hunters each have one or more chromosomes, which each have one or more cells. Now we shall look in each component in detail.

Cells The cells are the fundamental building block of the hunter. Each cell codes for a function, an upper and a lower limit, and a not flag. Each cell has the ability to vote on a sample, which is an array of some number of doubles, each of which must be $\epsilon[0, 1)$. When a cell votes on a sample, it is equivalent to saying, “feature f is [not] between lower limit and upper limit”. Where not is the not flag, and feature f is a particular entry in the sample. Lower and upper limits are each binary encoded reals, which use 8 bits each. The encoding is straightforward: the bits have all been shifted so that rather than the least significant bit being the 2^0 power, it is the 2^{-9} , allowing the most significant bit to be the 2^{-1} , giving each limit the ability to code for 0 to $\frac{511}{512} = 1 - 2^{-9} \cong .998$. This is why in preprocessing we squeeze values down so that they are attainable by Cells. The limits take 8 bits each, then the not flag takes another, and the feature bits take $\lceil \log_2(Features) \rceil$ bits

There is some error checking here, the lower limit bits cannot be greater than the upper limit bits, and so they’ll be swapped if that occurs. Also, the feature bits, unless there are a power of 2 features in the dataset will have illegal values. If these occur, all of the feature bits are rerolled randomly until compliant.

Finally, there is also a join bit whose purpose is simply whether or not to include the next cell in the vote. If the join bit is false, even if there are other cells to vote, then voting ends. This illustrates a breach in the chain, and is analogous to a form of gene regulation. More importantly, it allows genetic information to accumulate without affecting a particular Hunter’s vote. This sort of functionality, that is the ability to turn off a gene while it mutates and changes, has been shown in [Zhang \(2003\)](#) to be a critical component in gene duplication’s role in increasing informational complexity, and we hope to take advantage of a very powerful evolutionary mechanism by providing a means of doing so.

One other thing worth noting: as written, cells functions are one-to-one mappings as an index to a sample, but this doesn’t need to be the case. If a function can take an array of doubles and return a sensible value between 0 and 1, then it would fit into this piece of the puzzle. Most obviously, neural networks can fit this criteria; it would be

possible to, say, use an auto-encoder for feature extraction to get down to a certain number of features, and then use the feature index to extract one of those. This, however, would require a somewhat less generic approach than our thesis requires, as neural nets require extensive training and most of the datasets we're using are far too small. Coupling a simple neural net or two might to this algorithm might be one means of significantly increasing performance.

Chromosome Next, we have the chromosome, which is simply a sequence of one or more cells, with a few bits added. First are the class bits, which make up the first $\lceil \log_2(Classes) \rceil$ bits, and these mean that votes from cells in that chromosome count toward that class. Next are 2 affinity bits, which we will discuss in detail in Merger. In brief, they describe how the chromosome will behave with other chromosomes. Finally, a not flag, which inverts the votes of their cells.

Cells vote in sequence. Each vote is logically ANDed with the next. If at any point a vote is false, voting stops and false is returned. The Chromosome then takes this vote and passes it up to the Hunter which called it after inverting it if the not flag so dictates.

Hunter At the highest level of the critter hierarchy is the Hunter. Here, there are no additional bits, they simply aggregate the votes of their on or more chromosomes. We can now discuss explicitly the voting process.

2.4: Purist Voting Algorithms

```

1 Hunter.Vote(Sample x):
2     Counts[] := new Int[Classes]
3     for each Chromosome c in Chromosomes:
4         if Chromosome.Vote(x) == TRUE:
5             Counts[c.ClassBits.ToInt()] += 1
6     MaxIndex = HighestIndexOf(Counts)

```

```

7         return Counts[MaxIndex]
8
9 Chromosome.Vote(Sample x):
10     Result = TRUE
11     for each Cell c in Cells:
12         Result &= c.Vote(x)
13         if (Result == FALSE or c.JoinBit == FALSE)
14             break
15     return Result ^ NotFlag //Where ^ is Exclusive Or
16
17 Cell.Vote(Sample x):
18     Value = Functions[FunctionBits](x)
19     Result = Value > lowerLimit & Value < upperLimit
20     return Result ^ NotFlag

```

In case of a tie, Hunter returns the lowest index, and in case of no votes returns a -1, which represents uncertainty. Thus, as written voting is deterministic, and as such a Hunter's performance is determined entirely by its bitstring. This enables the cheap storage and recall of even very complicated Hunters.

Complexity is certainly an issue, but before we can discuss it we need to discuss how breeding operators can handle this new complexity. Either because with variable length genomes crossover can't work unmodified, or because complexity wouldn't increase past whatever was assigned at generation 0. Both of these cases could be true without modification of the typical GA.

First, we will discuss our modifications to the classical crossover operators. Here we differ from our inspiration for this portion of our paper ([Kharmah et al., 2004](#)). While their crossover operator is modified to accommodate different length genes, our crossover treats each collection of genetic material distinctly.

Crossover Our crossover is invoked at the hunter level. Any two hunters may be crossed. Crossover may occur at the level of swapping Chromosomes, or may go deeper, so that two Chromosomes can swap cells, or it can go deeper still, such that two cells can crossover as normal, since all cells are the same length. In the highest level case, the operation can be thought of as crossover with chromosomes laid out contiguously. In the event that hunters have a different number of chromosomes, the remainder are allocated randomly according to the crossover rate.

In the middle case, Chromosomes perform a similar function with cells. Cells are left untouched but are swapped back and forth, functioning similarly to bits in a standard crossover operation.

In the lowest case (which we call Uniform), the case we have implemented, there's crossing over at all levels. It is probably most easily seen in algorithm form.

2.5: Hunter Crossover

```
1 Hunter.Crossover(Hunter a, Hunter b):
2     target = new Hunter(), notTarget = new Hunter()//Empty hunters for
3         receiving genetic code
4     least = min(a.Chromosomes, b.Chromosomes)
5     most = max(a.Chromosomes, b.Chromosomes)
6     if(max = a.Chromosomes) MaxHunter = a
7     else MaxHunter = b
8     for i = 0 to least:
9         newChromosomes = Chromosome.CrossOver(a[i], b[i])
10        if (RNG.Next < CrossoverChance)
11            switchTargets(target, notTarget)
12            target.AddChromosome(newChromosomes[0])
13            notTarget.AddChromosome(newChromosomes[1])
14    for i = least to most:
```

```

14         if (RNG.Next < CrossoverChance)
15             switchTargets(target, notTarget)
16             target.AddChromosome(MaxHunter[i])
17     return target,notTarget;

```

One minor addition here is that target and notTarget are actually pointers to hunters (and below to Chromosomes), though it obfuscates the algorithm unnecessarily to spell that out in pseudocode, particularly because switch targets is intuitive even if not explicit. As you can see, this allows us to cross hunters of any length. The algorithm for Chromosomes is similar, except that unlike hunters they have genetic material of their own to cross. However, what should also be clear is that while different lengths of chromosomes and hunters might arise, there is no mechanism here to increase those lengths.

2.6: Chromosome Crossover

```

1  Chromosome.Crossover(Hunter a, Hunter b):
2      target = new Chromosome(), notTarget = new Chromosome()least =
        min(a.Cells, b.Cells)
3      most = max(a.Cells, b.Cells)
4      if(max = a.Chromosomes) MaxChromosome = a
5      else MaxChromosome = b
6
7      for i = 0 to ChromosomeBitLength:
8          target.bits[i] = a.bits[i];
9          notTarget.bits[i] = b.bits[i];
10         if (RNG.Next < CrossoverChance)
11             switchTargets(target, notTarget)
12
13         //Now that the chromosome specific bits are crossed, we may proceed
14         for i = 0 to least:
            newChromosomes = Chromosome.CrossOver(a[i], b[i])

```

```

15         if (RNG.Next < CrossoverChance)
16             switchTargets(target, notTarget)
17             target.AddChromosome(newChromosomes[0])
18             notTarget.AddChromosome(newChromosomes[1])
19     for i = least to most:
20         if (RNG.Next < CrossoverChance)
21             switchTargets(target, notTarget)
22             target.AddCell(MaxChromosome[i])
23     return target,notTarget;

```

Cell.Crossover is the usual implementation of uniform crossover. The lengths of Hunters and Chromosomes is something we refer to as complexity. Specifically, complexity is the number of Cells in a Hunter. So a Hunter with 2 Chromosomes with 1 Cell each and a Hunter with 1 Chromosome with 2 Cells have the same complexity for our purposes. With crossover and mutation, the complexity of a population will never increase beyond what is injected at the beginning. The combined complexity of a pair's offspring, further, can never increase with this method, it must remain the same.

To allow our algorithm to manipulate complexity on its own, we use the genetic operator Merger, first introduced in [Kharma et al. \(2004\)](#). When two Hunters merge, the result is a single Hunter with the sum of their complexities. To accomplish this, the Chromosomes of the Hunters need to be merged in some way. This is where the Affinity bits on the Chromosome come into play.

Merger In the broadest sense, Merger can be seen as combining the Chromosomes of two Hunters. One option would simply be to append the Chromosomes in one list to the other. But this would eventually yield many short Chromosomes, each with few cells. Instead, Merger uses Chromosomes' affinity to control how the merging is accomplished. First, recall that there are 2 affinity bits, resulting in 4 possible

a	b	Meaning
0	0	No preference.
0	1	Prefers to be at the rear.
1	0	Prefers to be at the front.
1	1	Considers itself complete.

Table 2.1: Interpretation of Affinity Bits

combinations. See table 2.1 for details.

When two chromosomes are merged, two outcomes are possible. First, both Chromosomes merge vertically, that is, they are both copied into the new Hunter next to each other in the list, retaining all distinguishing characteristics. Second, the Chromosomes merge horizontally, with one chromosome being the front and the other being the rear. The front Chromosome carries the class and affinity bits, the ones in the rear are destroyed. To determine which, compare the affinity bits of the 2 with an AND. This reveals where conflicts are: if the result is not 00, then the Chromosomes merge vertically. If the result is 00, the Chromosomes merge horizontally, with one exception: Chromosomes which consider themselves complete will always merge vertically. To determine which Chromosome goes in the front, we see which one has a preference. If there is none and there are no conflicts, Chromosome A goes to the front. To be more explicit, see table 2.2.

This allows for the growth of complexity in a nuanced way. However, in any of these cases, we have doubling complexity. This will easily lead to an explosion of complexity, since there is no mechanism which explicitly reduces complexity. Crossover serves to move complexity toward the average, and mutation ignores complexity altogether. The only one we have is implicit, that is, if complex individuals are less fit they will be removed from the breeding pool eventually. However, if they are more fit, then they are likely to double in complexity, etc. Because this is exponential growth, we must be careful to curb it. Exactly how we do this requires discussion of our fitness

A	B	Result
00	00	Laid out Horizontally with A in front
00	01	
10	00	
10	01	
00	10	Laid out Horizontally with B in front
01	00	
01	10	
11	**	Laid out Vertically
**	11	
10	10	
01	01	

Table 2.2: Merger Outcomes

function.

Fitness At the outset, our fitness function is the same as the one which we have discussed for our Optimizers, average accuracy, or \bar{A} . We reduce this with complexity, such that:

$$F_{Hunter} = \bar{A} \left(\frac{C_{Max} - C}{C_{Max}} \right)$$

where C_{Max} is the complexity cap and C is the Hunter’s complexity. C_{Max} is quite high, 2000, and we haven’t seen it reach the point where fitness become negative, however we still set negative fitness to 0. So this has a modest impact on fitness; most of the time it is multiplying by something fairly close to unity. Two Hunters with identical \bar{A} are likely to have different complexities, meaning the simpler one will get the edge when sorting. The other reason we adjust the fitness function goes all the way back to the mid-eighteenth century.

Specifically, all the way to Bach. Bach wrote many chorales, 4 part harmonies which each have a key. There are many possible keys, 103 in fact. In the formulation of the dataset as a classification problem, each key becomes a class and that means that we have a very sparse matrix of 103*103 to score. The problem is that chances of getting

any particular class correct is so unlikely that there's not much pressure to find new ways of doing it. So here, we tweak our fitness function again.

$$F_{Hunter} = \overline{A} \left(\frac{C_{Max} - C}{C_{Max}} \right) \left(\frac{E - Z}{E} \right)$$

In this last portion, E is the number of classes in the dataset, where Z is the number of classes for which the Hunter has made 0 predictions. Thus, if all of the predictions are in one or two classes, we are left with a high factor reducing the fitness of the Hunter. Likewise, hunters which make predictions in more classes will realize a bonus compared to their peers. This modification doesn't hurt convergence in datasets with smaller numbers of classes, and does help with Bach's chorales. We will discuss results in more detail in chapter 3. Earlier modifications were more stepwise and could even result in negative fitness, but these had little positive impact.

Daedalus All that remains for the purist approach is to discuss Daedalus⁸, the functional equivalent to Evolver for the Optimizers. Daedalus handles local constants and file IO. Unlike in Evolver, it is solely responsible for IO. Like Evolver, it captures metrics and runs a version of the standard GA which is pretty close to the canonical interpretation. Logically, it is almost identical to 2.3. We instead will focus on how the next generation is generated.

2.7: Daedalus Generate Next Generation

```

1 Daedalus.GenerateNextGeneration():
2     BreedingPop = StochasticUniformSample(P)
3     nextGen = Elitism(P)
4     FillListFromBreedingPop(nextGen, BreedingPop)
5     for i from P.Count*ElitePercent to P.Count:
6         nextGen[i].Mutate()
7     P = nextGen

```

⁸The initial idea was to have Daedalus as the trainer and Icarus as the Validator, but this was deemed unnecessary and validation was rolled into Daedalus.


```

8
9 Daedalus.FillListFromBreedingPop(nextGen, BreedingPool):
10     mergeList = List
11     for i from 0 to BreedingPool.Count:
12         if(RNG.NextDouble() < MergePercent) mergeList.Append(i)
13     used = mergeList.Set()//Don't want to pick other mergees
14     for each target in mergeList:
15         k = GetUnpickedInt(BreedingPop.Count, used)
16         used.Append(k)
17         nextGen.Add(Hunter.Merge(BreedingPop[target],
18                                 BreedingPop[k]))
19     while nextGen.Count < P.Count:
20         j = RNG.NextInt(0, ElitismPercent*BreedingPop.Count)
21         k = RNG.NextInt(0, BreedingPop.Count))
22         for each Hunter x in (Hunter.Crossover(BreedingPop[j],
23                                                 BreedingPop[k])):
24             nextGen.Add(x)
25     while nextGen.Count > P.Count:
26         nextGen.Pop()
27
28 GetUnpickedInt(Max, picked):
29     if(picked.Count >= Max) return -1
30     unpicked = RNG.Next(0, Max)
31     while picked.Contains(unpicked):
32         unpicked = RNG.Next(0, Max)
33     return unpicked

```

A few things worth noticing in this algorithm: Merge is executed first, and all Hunters in the breeding pool get a chance at merging, and an effort is made to prevent any particular Hunter from merging more than once. Used (and picked in

GetUnpickedInt()) are Sets, which only retain the first copy of any element added to them. While not strictly necessary for this algorithm, there are other cases where duplicate entries are more likely and GetUnpickedInt was already implemented with Sets. Also, breeding takes place until the next generation is the same size as the original population, so this method is resilient to changes to Crossover and Merge, and errors in case there were inviable offspring, which is not an issue with our implementation but a cautionary design principle to keep that as a possible change. One major difference between Daedalus and Evolver’s mode of advancing generation is that Daedalus incorporates validation into its algorithm. That is, every time time data will be written to disk (in our case, every 25 generations), the entire population is evaluated, sorted, and bred based on the validation dataset, which is identical to the testing set for the Optimizers. The idea is to drive evolution using the training set, and occasionally course-correct with the validation set. Where classifiers have a distinct, defined method for doing this (for instance, Bayes building a model from the training set), with GAs the evolution *is* the method of learning. Similarly, because this additional time is necessary, the Purist Approach takes 10 times as many generations, and has a larger population by a similar factor, to the Optimizers. Also, because Daedalus is native, we can make use of multi-threading to improve processor efficiency.

The last thing worth noting about Daedalus is that its starting condition has a few criteria that are different to it than the Optimizers. First, each Hunter is given E (where E is the number of classes in the data) Chromosomes to begin with, at 1 cell each. The class bits are then initialized to count from 0 to E, so that it is guaranteed to have a Chromosome voting for each of the classes. While we recognize that this might be seen as ad hoc tweaking⁹, it is rooted in strong intuitions about this algorithm and its shortcomings. While we don’t have the data any longer, it managed to get the Hunters working on the Bach dataset over a considerable hump.

In this chapter, we have discussed in detail how our algorithms work. We explained

⁹Or Alchemy.

how to configure a dataset to work with our methods. We described the changes we need to make to the dataset before we pass it to the programs responsible for them, whether they are external or internal. We then discussed the theoretical underpinnings of two different classifiers which we then optimize 2 ways each, and finally discussed our own purist approach. Next, we will discuss the results of our implementations.

Chapter 3

Results

In this chapter, we will briefly describe the datasets tested and the results of our experiments. We will then discuss our findings, looking at the confusion matrices and focusing on four metrics: Accuracy, Average Accuracy (\bar{A}), Matthew's Correlation Coefficient (MCC) and Confusion Entropy. We came to MCC and CEN later in the project, but they provide some insight into multidimensional confusion matrices. A brief introduction to the two metrics follows.

MCC is a real valued number between -1 and 1, and is equivalent to

$$\frac{cov(X, Y)}{\sqrt{cov(X, X) \cdot cov(Y, Y)}}$$

The magnitude measures the amount of information not attributable to random chance. A 1 is a perfect correlation with the data, only achievable when accuracy is also equal to 1. A -1 is a perfect anti-correlation, though generating it is not as simple as merely getting everything wrong. Finally, a 0 means that the prediction is performing no better than chance. For further information, we recommend [Jurman et al. \(2012\)](#).

[Wei et al. \(2010\)](#) contains the full detail and motivation regarding CEN, which ranges from 0 to 1. In this case, 0 indicates a perfect matrix, and 1 virtually no self-information. To be crude but generally accurate, CEN is a measure of the probability

of misclassification of classes by the classifier. Thus, lower is better. We calculate it as

$$CEN = - \sum_j^{N+1} P_j \sum_k^{N+1} P_{j,k}^j \log_N(P_{j,k}^j) + P_{k,j}^j \log_N(P_{k,j}^j)$$

$$P_{i,j}^i = \frac{C_{i,j}}{\sum_{k=1}^{N+1} C_{i,k} + C_{k,i}}$$

$$P_{i,j}^j = \frac{C_{i,j}}{\sum_{k=1}^{N+1} C_{j,k} + C_{k,j}}$$

$$P_j = \frac{\sum_{k=1}^{N+1} C_{j,k} + C_{k,j}}{2 \sum_{k,l}^{N+1} C_{k,l}}$$

Where C is the confusion matrix. P_j is the probability of misclassifying a particular class, $P_{i,j}^i$ is the probability of misclassifying ω_i as ω_j subject to class i, and $P_{i,j}^j$ is the same, but subject to class j. To understand this, pay particular attention to the denominators where the classes sum over different "crosses", centered at the superscripted variable which is fixed, while k iterates both horizontally and vertically across the matrix. Also, for calculation purposes, $P_{i,i}^i = 0$, and logs of 0 in the density function may also be treated as 0.

3.1 Datasets

All of our datasets were acquired from the UCI database (Lichman, 2013). We used 3 different datasets, trying to span multiple fields of study. To that end we used Yeast (Paul Horton, 1996), which is a relatively simple biological dataset,

Cardioctocography (J. P. Marques de S et al., 2010) (Cardio) which is a medical dataset, and Bach’s Chorales (Daniele P. Radicioni and Roberto Esposito, 2014) which is a musical dataset. With minimal configuration, described in Chapter 2, our program can handle virtually any dataset in the standard matrix form. We will first describe the makeup of the dataset, provide a visualization of the data through a method called t-distributed stochastic neighbor embedding(T-SNE) first developed in Maaten and Hinton (2008).

T-SNE is conceptually similar to K-Nearest Neighbors, in that it is unsupervised and assumes that things which are similar will be nearby in whatever n-dimensional space they are embedded in. Indeed, T-SNE takes the distances of each point to all other points and converts them to probabilities, then builds probability density functions maximizing their likelihood. The density functions in this case are student-T distributions, which are similar to Gaussian distributions but their tails are much fatter; that is, they don’t go to zero nearly as quickly. Once these distributions are built T-SNE iteratively performs a form of gradient descent minimizing the error of the predictions of the T distributions. It is very good at maintaining separability found at high dimensions into lower-dimensional spaces, which makes it good for plotting. However, there are concerns that it may not be particularly good at doing dimensional reduction, which often means a reliance on Principal Component Analysis or some similar method to handle that portion(Maaten and Hinton, 2008).

Yeast Dataset This dataset is used to predict the localizations of proteins in a yeast’s cell. Its meanings and usage are fully motivated in Nakai and Kanehisa (1992). For our purposes, each sample (of 1484) belong to one of 10 classes, which correlate to their function within the cell. The original paper used an expert system which boasted 59% accuracy. For a visualization of Yeast, see figure 3.1. This should be the best case scenario. There are very few features, and a handful of classes, so

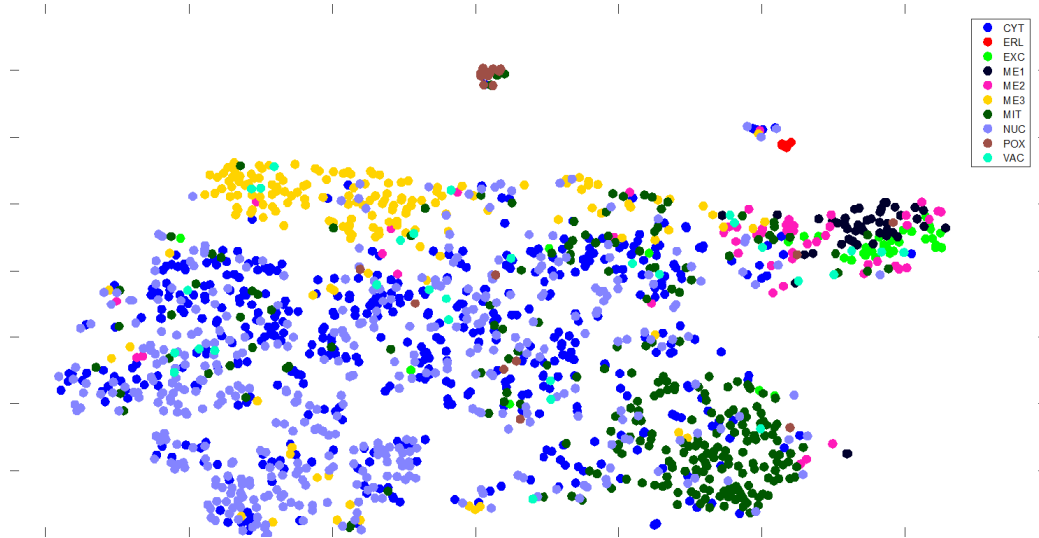


Figure 3.1: T-SNE visualization of Yeast dataset. Viewing in color is highly recommended.

barring inseparable data (which the visualization demonstrates to not be the case) there should be little trouble for a classifier to find some signal in the data.

Cardiotocography Dataset Cardiotocography is the practice of monitoring fetal heartbeats during pregnancy. The Cardiotocograph (CTG) is the machine used to monitor, and it produces cardiotocograms. The dataset is based on [Ayres-de campos et al. \(2000\)](#) and was also used, in limited form, in [Ocak \(2013\)](#), where the researchers achieved an impressive 100% specificity (in this case, the correct classification of pathologic cardiotocograms). Their sensitivity was also very high: 99.3% on the training set. Clearly here specificity is more important than sensitivity! Unfortunately, these researchers left out approximately 200 samples of suspicious cardiotocograms, which confound things considerably. There are good methodological reasons for doing this, of course. SVMs don't work as well with more than 2 classes, and culturally medicine is very concerned with sensitivity and specificity, which don't apply to non-binary problems in general. We certainly aren't criticizing the good work medical researchers do, nor the lives they save.

We do include the suspect cardiotocograms, so we don't expect our results to be quite

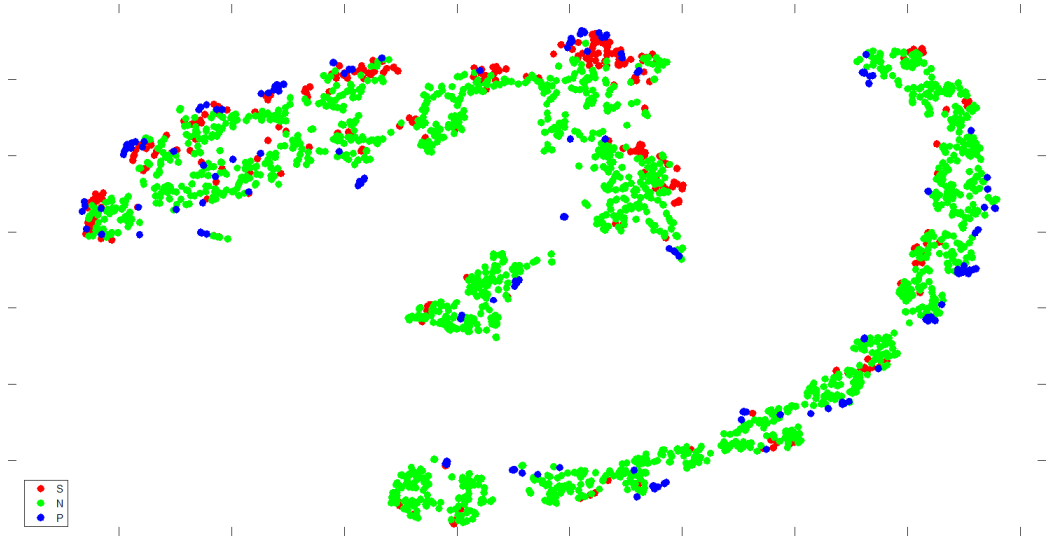


Figure 3.2: T-SNE visualization of Cardio dataset, following the NSP classification schema.

as clean. Further, there are two classification modes in this dataset, not 1. The first is what we’ve mentioned already, the Normal, Suspect, Pathologic (NSP) classifications. The second is the morphologic patterns 1-10. These may or may not overlap with the NSP, but they provide a second way of looking at the data and evaluating it. We have provided T-SNE visualizations with both colorings below in 3.2 and 3.3.

Bach’s Chorales Bach composed all manner of music, but this dataset comprises 58 of his 4 part harmonies, called Chorales. Originally made a dataset in Radicioni and Esposito (2010) the music of 58 chorales are painstakingly broken into 5665 musical moments, such that every time there are 3 or more distinct notes being played it their proper key is classified, but there are confounding factors. Primarily, there might be added notes, which means a note must always be taken in context, which makes the problem much more difficult. What was a fairly modest 36 classes (12 notes \times 3 modes) becomes 108 when added notes are taken into account. Originally the authors used a perceptron which scored 75% accuracy, which is certainly much better than chance because, while there are 108 possible classes, only 102 can actually be found in the dataset.

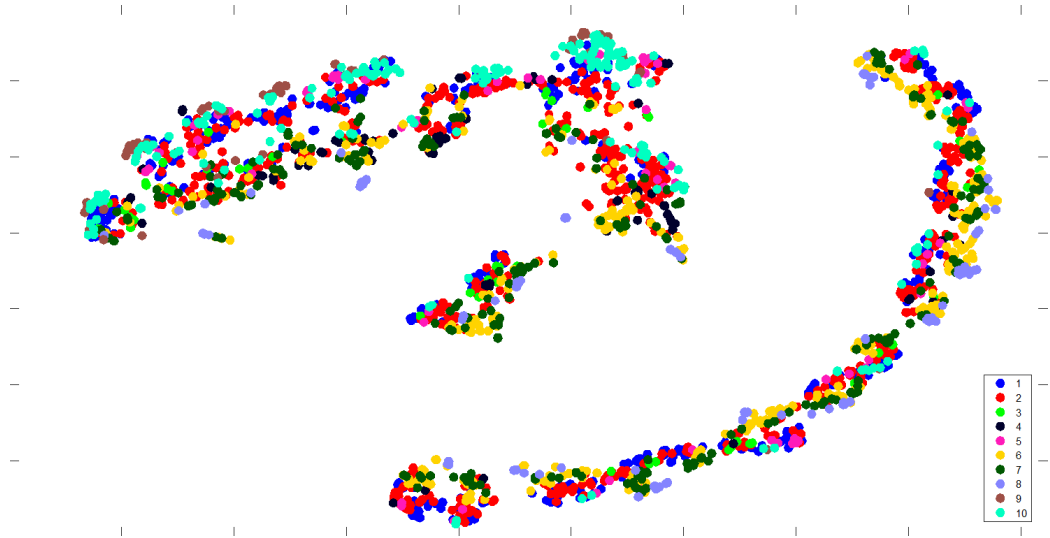


Figure 3.3: T-SNE visualization of Cardio dataset, following the 10-class morphology schema. Viewing in color is highly recommended.

We should note that we modified this dataset slightly. Initially they were published in the order in which they occurred. We added an additional feature including the key of the previous event and then randomized the order of the file before splitting it into training and testing sets. The hopes were that our algorithms would be able to take advantage of the temporal information in their models, even if they weren't explicitly instructed that it was temporal. The visualization (3.4) is difficult to read because of the many classes, but clearly delineates several inherent clusters.

3.2 Results

3.2.1 Yeast

CTree Baseline : As we can see, the baseline did fairly well regarding the 3 most common classes, but its ability to distinguish the less frequent classifications suffered giving it a final \bar{A} of 64.1%, or an overall accuracy of 74.6%. See table 3.1 for more detail.

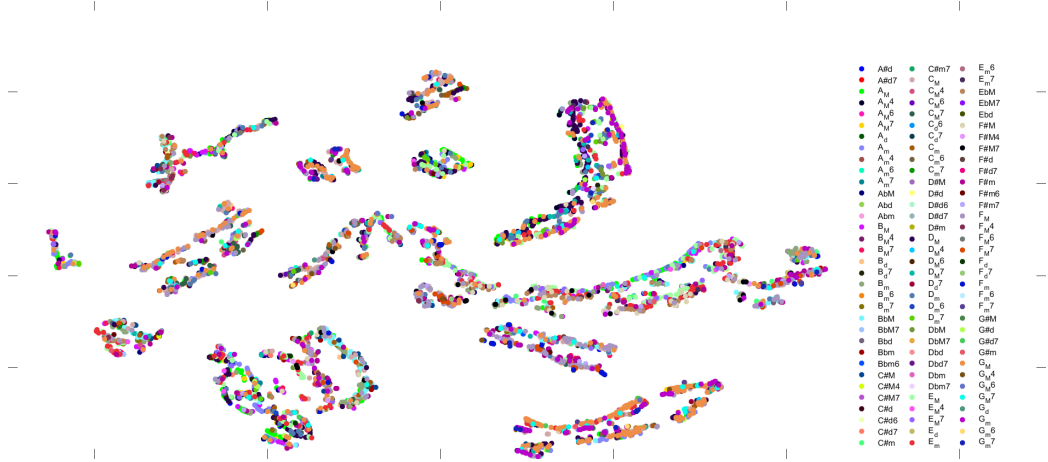


Figure 3.4: T-SNE visualization of 102 class Bach dataset. Classes are incredibly difficult to distinguish, but instead focus on the overall shapes and distinct clusters.

Class	MIT	NUC	CYT	ME1	EXC	ME2	ME3	VAC	POX	ERL	Total
MIT	151	14	24	0	0	5	2	1	1	1	199
NUC	8	145	36	0	1	0	4	1	3	0	198
CYT	19	30	133	0	3	4	1	2	5	1	198
ME1	1	0	0	14	2	1	0	0	0	0	18
EXC	0	0	0	0	12	0	0	0	0	0	12
ME2	0	1	1	2	1	21	0	0	0	0	26
ME3	1	4	3	1	0	2	67	0	0	0	78
VAC	0	1	0	0	0	0	0	1	0	0	2
POX	0	0	1	0	0	0	0	0	5	0	6
ERL	0	0	0	0	0	0	0	0	0	3	3
Total:	180	195	198	17	19	33	74	5	14	5	740
TPR:	0.839	0.744	0.672	0.824	0.632	0.636	0.905	0.2	0.357	0.6	0.641

Table 3.1: Yeast Dataset, Classification Tree with all features included, Accuracy = 74.6%, MCC: 0.674 CEN: 0.273

CTree w/ feature selection : With feature selection \bar{A} increased modestly to 65.8%, but accuracy declined to 68.4%. See table 3.2.

McNB Baseline With all features, \bar{A} was quite good: 85.9%. However, overall accuracy was 72.8%. See table 3.3 for confusion matrix and other details.

Class	MIT	NUC	CYT	ME1	EXC	ME2	ME3	VAC	POX	ERL	Total
MIT	131	13	9	0	0	1	2	0	2	0	158
NUC	8	87	26	0	1	0	1	2	0	0	125
CYT	33	87	158	0	3	2	4	2	4	0	293
ME1	1	0	0	13	2	1	0	0	0	0	17
EXC	1	0	0	1	11	1	0	0	0	0	14
ME2	5	2	1	2	2	26	0	0	0	1	39
ME3	1	5	3	1	0	2	67	0	0	0	79
VAC	0	1	0	0	0	0	0	1	0	0	2
POX	0	0	1	0	0	0	0	0	8	0	9
ERL	0	0	0	0	0	0	0	0	0	4	4
Total:	180	195	198	17	19	33	74	5	14	5	740
TPR:	0.728	0.446	0.798	0.765	0.579	0.788	0.905	0.2	0.571	0.8	0.658

Table 3.2: Yeast Dataset, Classification Tree with feature selection, Accuracy = 68.4%, MCC: 0.607 CEN: 0.290

Class	MIT	NUC	CYT	ME1	EXC	ME2	ME3	VAC	POX	ERL	Total
MIT	119	10	10	0	0	0	1	0	1	0	141
NUC	9	108	17	0	0	1	0	0	0	0	135
CYT	18	35	152	0	1	0	0	1	0	0	207
ME1	4	4	2	17	0	0	0	0	0	0	27
EXC	4	6	2	0	18	0	0	0	0	0	30
ME2	12	9	5	0	0	32	2	0	0	0	60
ME3	8	10	5	0	0	0	71	0	0	0	94
VAC	1	5	0	0	0	0	0	4	0	0	10
POX	5	8	5	0	0	0	0	0	13	0	31
ERL	0	0	0	0	0	0	0	0	0	5	5
Total:	180	195	198	17	19	33	74	5	14	5	740
TPR:	0.661	0.554	0.768	1	0.947	0.97	0.959	0.8	0.929	1	0.859

Table 3.3: Yeast Dataset, Multiclass Naïve Bayes with all features included, Accuracy = 72.8%, MCC: 0.671 CEN: 0.293

McNB w/ feature selection: With feature selection, Multiclass Naïve Bayes had the highest \bar{A} of 87%, though with an accuracy of only 72.8%. The disparity is accounted for in the accuracy across the first 3 classes, which make up more than $\frac{3}{4}$ of the dataset. On them, accuracy ranged between abysmal and mediocre. We can clearly see the danger of a highly skewed dataset and the dangers of metrics than are

do not take this sufficiently into account. See table 3.1 for details.

Class	MIT	NUC	CYT	ME1	EXC	ME2	ME3	VAC	POX	ERL	Total
MIT	124	22	17	0	0	0	0	0	1	0	164
NUC	8	90	21	0	0	0	0	0	0	0	119
CYT	13	36	134	0	1	0	0	0	0	0	184
ME1	3	1	1	17	0	0	0	0	0	0	22
EXC	2	3	1	0	18	0	0	0	0	0	24
ME2	9	8	4	0	0	33	0	0	0	0	54
ME3	15	20	12	0	0	0	74	0	0	0	121
VAC	2	9	3	0	0	0	0	5	0	0	19
POX	4	5	5	0	0	0	0	0	13	0	27
ERL	0	1	0	0	0	0	0	0	0	5	6
Total:	180	195	198	17	19	33	74	5	14	5	740
TPR:	0.689	0.462	0.677	1	0.947	1	1	1	0.929	1	0.87

Table 3.4: Yeast Dataset, Multiclass Naïve Bayes with feature selection included, Accuracy = 72.8%, MCC: 0.630 CEN: 0.310

Hunter The Hunter underperformed the four other methods by any measure, and took a great deal (more than 100 times) more processor time to do it. This was supposed to be the best case for the Hunters, and early indications say that it is. $\bar{A} = .473\%$, while accuracy is 51.1%. Table 3.5.

Which classifier performed best is open for debate, both CTree and McNB are promising in their own ways. CTree seems to do a better job with the bulk classes, and perhaps if you’re optimizing average accuracy that’s a good way to go; optimize a method for something it is less suited for, resulting in a kind of check on optimization gone awry. Alternatively, perhaps the status of the major classes aren’t as important, and the focus instead is on discriminating between the outlying classes. In that case, McNB clearly wins. In any case, the Hunter didn’t do well, exactly, and with more time it might have done better, but that applies to any of these methods. The

Class	MIT	NUC	CYT	ME1	EXC	ME2	ME3	VAC	POX	ERL	Total
MIT	105	17	12	0	0	0	0	0	0	0	134
NUC	2	37	10	1	0	1	3	0	0	0	54
CYT	43	94	142	0	5	3	2	1	10	0	300
ME1	4	1	0	8	1	3	7	0	0	0	24
EXC	9	2	3	0	9	7	0	0	2	0	32
ME2	1	9	6	6	4	12	1	1	0	2	42
ME3	14	5	11	2	0	6	58	1	0	0	97
VAC	2	28	13	0	0	1	3	2	0	0	49
POX	0	0	1	0	0	0	0	0	2	0	3
ERL	0	2	0	0	0	0	0	0	0	3	5
Total:	180	195	198	17	19	33	74	5	14	5	740
TPR:	0.583	0.19	0.717	0.471	0.474	0.364	0.784	0.4	0.143	0.6	0.473

Table 3.5: Yeast Dataset, Hunter Accuracy = 51.1%, MCC: 0.413 CEN: 0.409

difference is that the Hunter already had 10 times as many generations and still didn't manage to get anywhere even close to competitive.

3.2.2 Cardiotocography NSP

CTree Baseline A classification tree handily gets 94% accuracy on this dataset, but that will prove to be a fairly unsurprising given this dataset. See table 3.6 for more details.

Class	Normal	Suspect	Pathologic	Total
Normal	519	31	9	559
Suspect	12	408	0	420
Pathologic	10	0	74	84
Total:	541	439	83	1063
TPR:	0.959	0.929	0.892	0.927

Table 3.6: Cardio Dataset, NSP Labels Classification Tree without feature selection included, Accuracy=94.1%, MCC: 0.967 CEN: 0.043

CTree w/ Feature Selection With feature selection, we see a similar pattern to yeast. Overall accuracy drops slightly, but the smaller classes get more accurate.

What’s interesting here is that MCC and CEN both decrease; see table 3.7 for more details.

Class	Normal	Suspect	Pathologic	Total
Normal	514	34	3	551
Suspect	12	405	0	417
Pathologic	15	0	80	95
Total:	541	439	83	1063
TPR:	0.95	0.923	0.964	0.946

Table 3.7: Cardio Dataset, NSP Labels Classification Tree with feature selection included, Accuracy: 93.9% MCC: 0.962 CEN: 0.051

McNB Baseline We get an accuracy of 90.2%, which is low compared to the previous classifiers, and the supporting metrics of MCC and CEN are much worse as well. See table 3.8 for details.

Class	Normal	Suspect	Pathologic	Total
Normal	476	24	6	506
Suspect	37	408	2	447
Pathologic	28	7	75	110
Total:	541	439	83	1063
TPR:	0.88	0.929	0.904	0.904

Table 3.8: Cardio Dataset, NSP Labels Multiclass Naïve Bayes without feature selection included, Accuracy = 90.2% MCC: 0.797 CEN: 0.186

McNB w/ Feature Selection Here, McNB manages to redeem itself somewhat. \overline{A} is the highest for any of the classifiers, and accuracy is only slightly lower than the baseline CTree. However, MCC and CEN are considerably worse than that tree, so take this classifiers’ predictions with a grain of salt.

Hunter This is probably the best we will see from the Hunter. That said, it didn’t do very well for the purpose of the dataset, which is distinguishing pathologic patterns from safe ones. See table 3.10 for further discussion.

Class	Normal	Suspect	Pathologic	Total
Normal	490	11	1	502
Suspect	28	427	0	455
Pathologic	23	1	82	106
Total:	541	439	83	1063
TPR:	0.906	0.973	0.988	0.956

Table 3.9: Cardio Dataset, NSP Labels Multiclass Naïve Bayes with feature selection included, Accuracy = 94%, MCC: 0.889 CEN: 0.116

Class	Normal	Suspect	Pathologic	Total
Normal	197	77	10	284
Suspect	183	322	4	509
Pathologic	161	40	69	270
Total:	541	439	83	1063
TPR:	0.364	0.733	0.831	0.643

Table 3.10: Cardio Dataset, NSP Labels Hunter, Accuracy = 55%, MCC: 0.333 CEN: 0.568

As we can see, the CTree without feature selection performed best on this dataset. For one thing, the dataset was developed by experts and they selected features that would be most indicative of problems. Also, it might seem strange that MCC and CEN were so much lower on the Bayesian classifiers. In examining the tables, pay close attention to how well the total in the right column matches the total in the row, and that should give an idea of why. In some sense, MCC and CEN are measures of the useful information from the classifier. In this case, when it makes a prediction of a particular class it's extremely confident. That's much more useful than what the Bayesian classifiers discern, *even though they get more of the pathological cases correct*. Because even though the McNB with feature selection gets 82 of the 83 pathological cases, it also misclassified them about 20% of the time.

3.2.3 Cardiotocography Morphology

CTree Baseline Again, this dataset proves to be highly separable, and CTree continues to do quite well. See table 3.11 for details.

Class	J	F	A	H	G	B	D	I	E	C	Total
J	97	0	2	0	0	0	0	0	2	0	101
F	0	159	0	1	5	6	0	0	0	0	171
A	4	0	183	0	0	5	0	0	1	1	194
H	0	0	0	42	2	0	1	0	0	2	47
G	0	1	1	0	120	1	0	0	0	0	123
B	0	0	1	0	0	286	3	0	3	1	294
D	0	1	0	0	0	1	38	0	0	0	40
I	3	0	1	0	0	0	0	28	0	0	32
E	2	0	5	0	0	1	0	0	31	1	40
C	0	0	2	0	0	0	0	0	0	19	21
Total:	106	161	195	43	127	300	42	28	37	24	1063
TPR:	0.915	0.988	0.938	0.977	0.945	0.953	0.905	1	0.838	0.792	0.925

Table 3.11: Cardio Dataset, Morphological Labels Classification Tree without feature selection included, Accuracy = 94.3% MCC: 0.933, CEN: 0.086

CTree w/ Feature Selection Compared to the baseline, accuracy increased marginally but MCC got slightly worse. CEN stayed the same to 3 significant figures. See table 3.12.

McNB Baseline Here, we again see the discriminative power of the Bayesian method: accuracy is up to 96% and CEN is down a full 3.5 points and MCC is up by almost the same. There's one class, I, where 100% of the cases were caught, that is, one perfect column, though there's no corresponding perfect row. See table 3.13.

McNB w/ Feature Selection This is the best we'll likely see from McNB: there are 3 perfect columns and 3 rows, and they overlap on 2 of the classes (I and H). Accuracy and \bar{A} are 98.3 and 98.1%, respectively, MCC is 0.980 and CEN is 0.030. See table 3.14 for further details.

Hunter This hunter actually manages a negative MCC, which represents it performing worse than chance. In some sense, this means that if this classifier says something you're better off picking *anything else* at random. See table 3.15 for details of its lackluster performance.

Class	J	F	A	H	G	B	D	I	E	C	Total
J	98	0	0	0	0	0	0	0	2	1	101
F	0	161	1	1	1	7	0	0	0	0	171
A	6	0	178	0	0	4	0	1	3	2	194
H	0	0	2	44	0	0	1	0	0	0	47
G	0	4	1	0	118	0	0	0	0	0	123
B	0	1	3	0	0	283	3	0	4	0	294
D	0	1	0	0	0	0	39	0	0	0	40
I	3	0	0	0	0	0	0	29	0	0	32
E	1	0	5	0	0	0	0	0	33	1	40
C	0	0	2	0	0	0	0	0	0	19	21
Total:	108	167	192	45	119	294	43	30	42	23	1063
TPR:	0.907	0.964	0.927	0.978	0.992	0.963	0.907	0.967	0.786	0.826	0.922

Table 3.12: Cardio Dataset, Morphological Labels Classification Tree with feature selection included accuracy: 94.3% MCC: 0.931, CEN: 0.086

Class	J	F	A	H	G	B	D	I	E	C	Total
J	99	0	2	0	0	0	0	0	0	0	101
F	0	169	0	0	0	1	0	0	0	1	171
A	2	0	189	0	0	2	0	0	0	1	194
H	0	0	0	47	0	0	0	0	0	0	47
G	0	1	0	1	121	0	0	0	0	0	123
B	0	5	9	0	2	276	1	0	1	0	294
D	0	0	0	0	0	0	40	0	0	0	40
I	2	0	0	0	0	0	0	30	0	0	32
E	2	0	0	0	0	0	0	0	38	0	40
C	0	0	0	0	0	0	0	0	0	21	21
Total:	105	175	200	48	123	279	41	30	39	23	1063
TPR:	0.943	0.966	0.945	0.979	0.984	0.989	0.976	1	0.974	0.913	0.967

Table 3.13: Cardio Dataset Morphological Labels Multiclass Naïve Bayes without feature selection, Accuracy= 96.9% MCC: 0.963, CEN: 0.05

3.2.4 Bach's Chorales

Unfortunately, there's not a good way of fitting a 103 index square confusion matrix on a single page that preserves readability. Thus, we have included instead heatmaps of the classifiers instead. We will discuss them as normal.

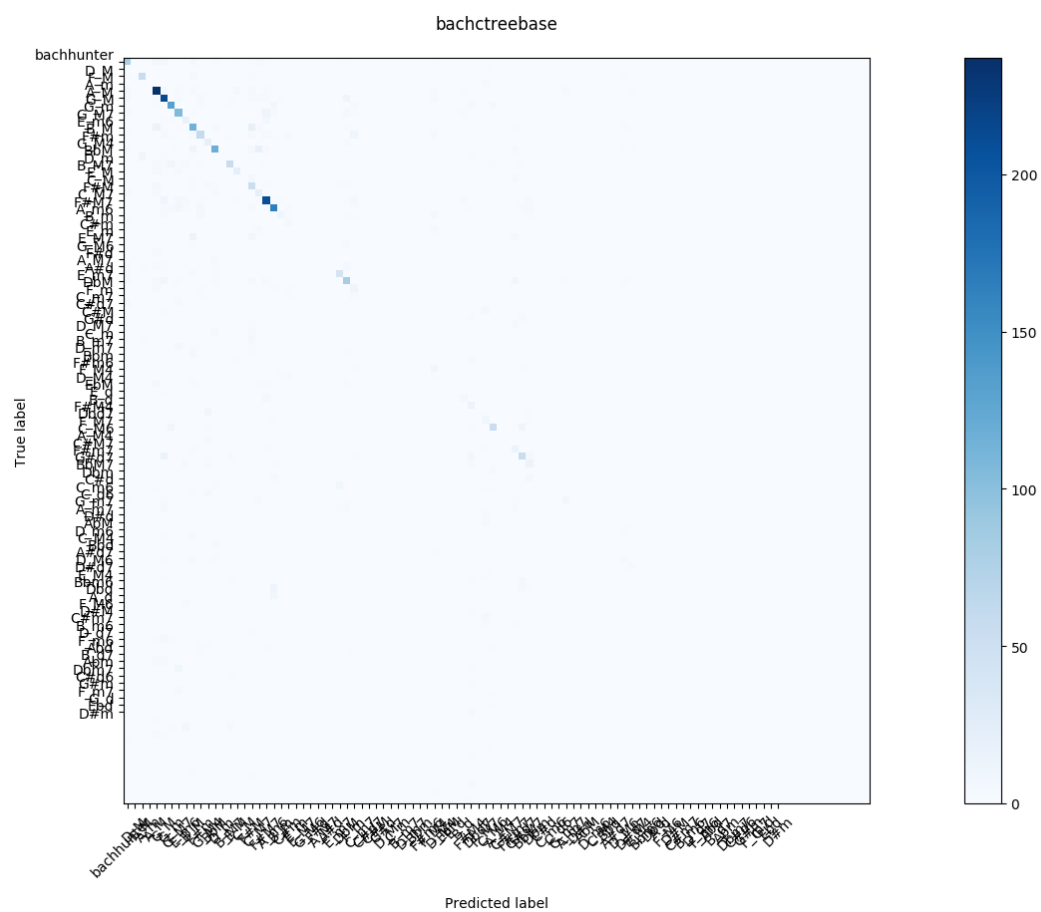


Figure 3.5: Bach's, CTree Baseline. Accuracy = 70.9%, $\bar{A} = 24.4\%$, MCC = 0.694
CEN = 0.18.

Class	J	F	A	H	G	B	D	I	E	C	Total
J	100	0	1	0	0	0	0	0	0	0	101
F	0	171	0	0	0	0	0	0	0	0	171
A	0	0	187	0	1	4	0	0	1	1	194
H	0	0	0	47	0	0	0	0	0	0	47
G	0	1	0	0	122	0	0	0	0	0	123
B	0	4	2	0	1	285	1	0	1	0	294
D	0	0	0	0	0	0	40	0	0	0	40
I	0	0	0	0	0	0	0	32	0	0	32
E	0	0	0	0	0	0	0	0	40	0	40
C	0	0	0	0	0	0	0	0	0	21	21
Total:	100	176	190	47	124	289	41	32	42	22	1063
TPR:	1	0.972	0.984	1	0.984	0.986	0.976	1	0.952	0.955	0.981

Table 3.14: Cardio Dataset Morphological Labels Multiclass Naïve Bayes with feature selection, Accuracy = 98.3%, MCC: 0.98, CEN: 0.03

Class	J	F	A	H	G	B	D	I	E	C	Total
J	28	19	0	1	21	0	3	2	27	0	101
F	0	5	0	0	2	163	1	0	0	0	171
A	16	86	10	0	33	5	1	40	1	2	194
H	0	1	0	38	4	3	0	1	0	0	47
G	0	43	0	1	65	3	10	1	0	0	123
B	2	3	0	0	2	284	1	2	0	0	294
D	0	0	0	0	0	40	0	0	0	0	40
I	0	6	0	16	0	0	0	10	0	0	32
E	9	7	0	0	12	0	0	8	4	0	40
C	0	11	0	0	3	0	1	6	0	0	21
Total:	55	181	10	56	142	498	17	70	32	2	1063
TPR:	0.509	0.028	1	0.679	0.458	0.57	0	0.143	0.125	0	0.351

Table 3.15: Cardio Dataset Morphological Labels Multiclass Naïve Bayes with feature selection, Accuracy = 41.7%, MCC: -0.078, CEN: 0.49

CTree Baseline CTree had some difficulty with this dataset. MCC was decent at 0.694, CEN seemed to be relatively good at 0.18. However, accuracy was 70.9%, which seems like decent performance (the perceptron in the original paper got 75%, after all), and the MCC seems to indicate this result is from some consolidation of signal rather than chance. \bar{A} is very low at 24.4%, but with so many classes that is not particularly surprising.

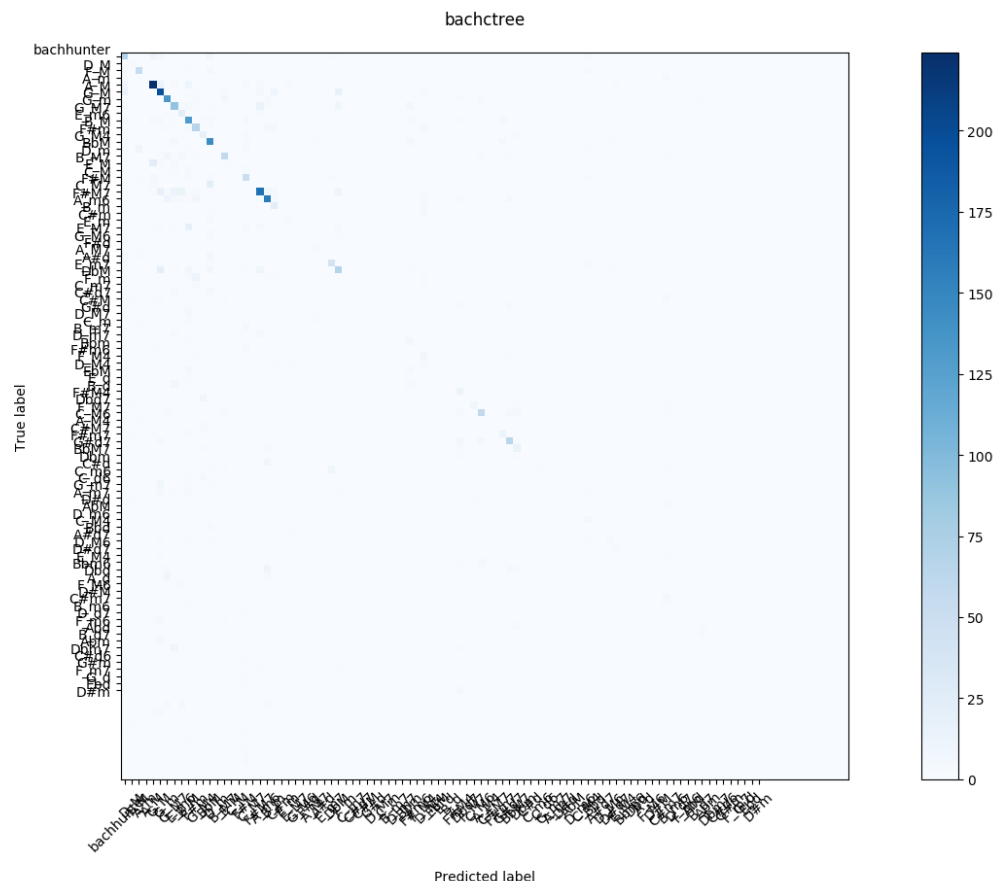


Figure 3.6: Bach’s, CTree. Accuracy = 67.9%, \bar{A} = 27.0%, MCC = 0.662 CEN = 0.192.

CTree w/ Feature Selection Unusually, performance decreased by most metrics here. That might be indicative that all dimensions are important to this set, which makes sense for music; it would be hard to discern the difference between two chords if you ignore a single key which contributes to one and not the other. This pattern doesn’t hold with the Bayesian classifier. Accuracy is 67.9%, while \bar{A} is 27.0%. MCC was 0.662, and CEN was 0.192.

McNB Baseline Here, we see a marked difference in performance between CTree and McNB. MCC at 0.785 is noticeably higher, and CEN at 0.139 is lower by about the same margin, and accuracy beats the original paper at 79.4%. \bar{A} is the biggest difference, though, and nearly triples the baseline CTree’s result at 66.2%.

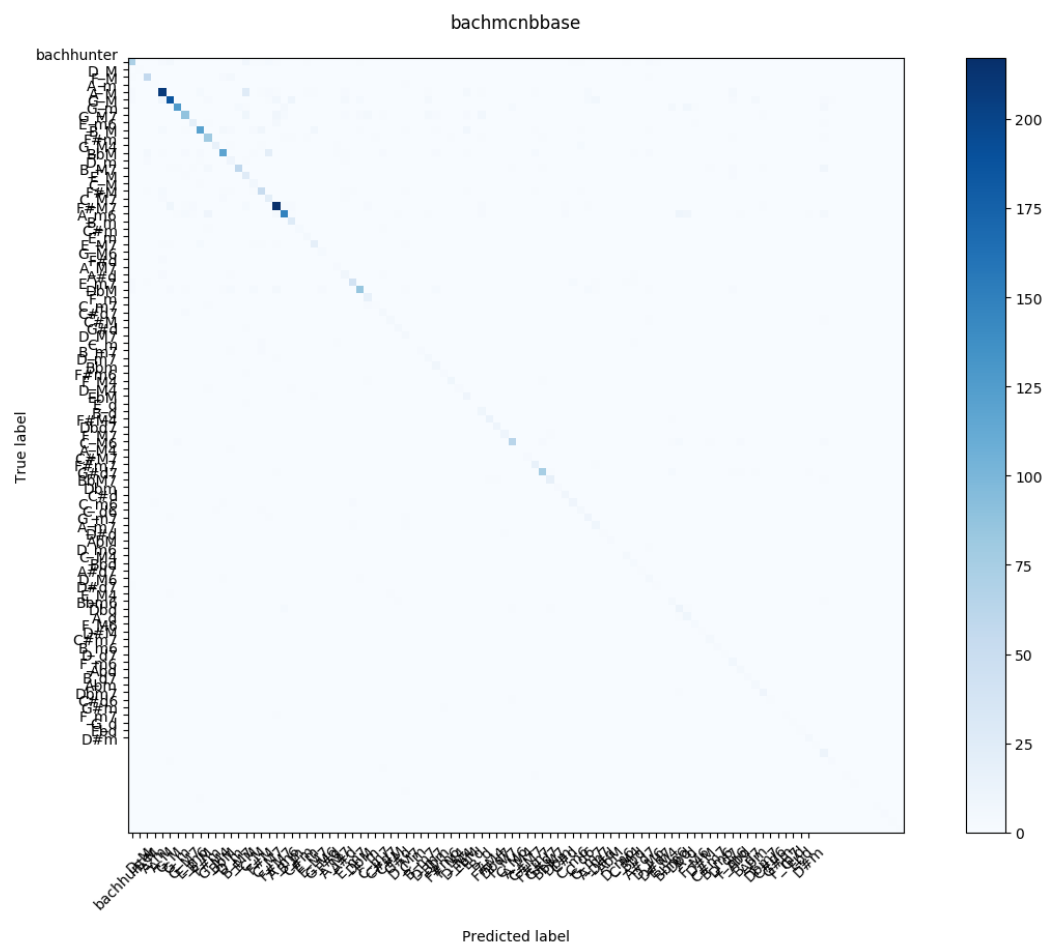


Figure 3.7: Bach's, McNB Baseline. Accuracy = 79.4%, $\bar{A} = 66.2\%$, MCC = 0.785
CEN = 0.139.

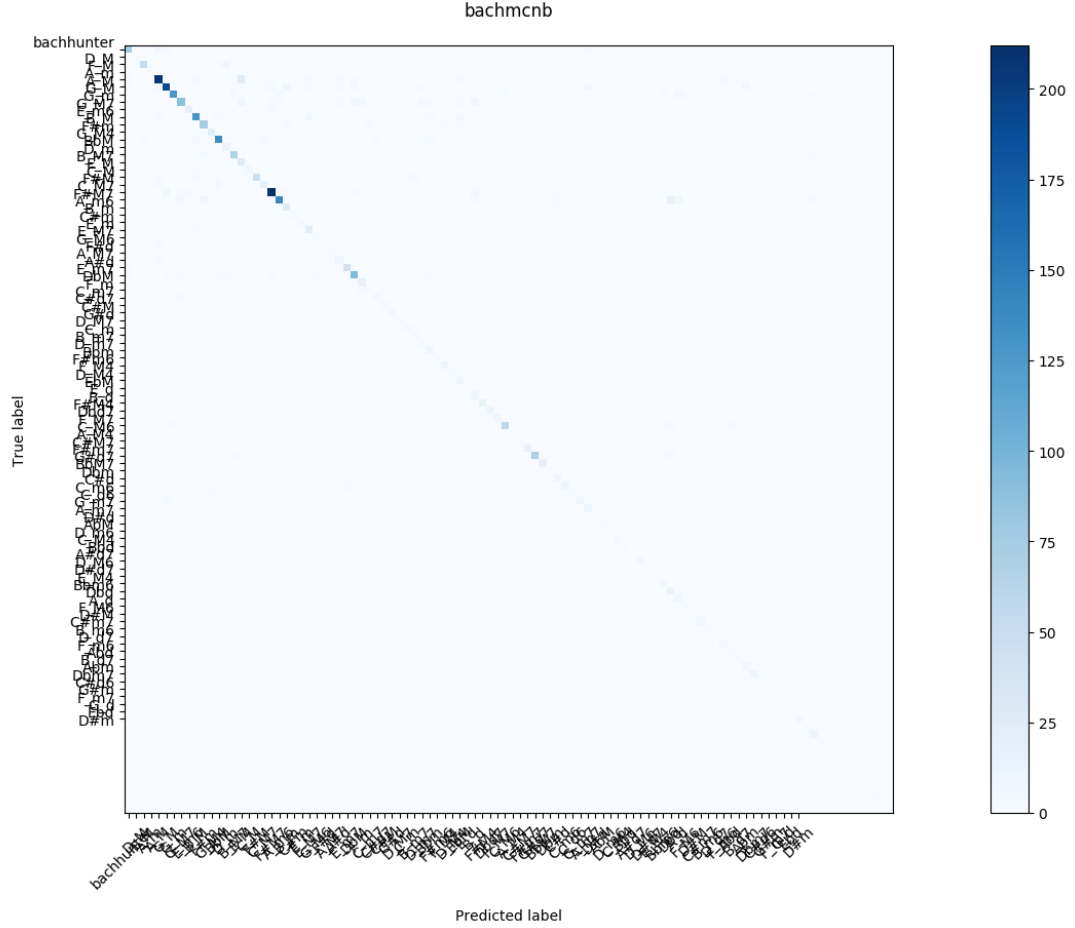


Figure 3.8: Bach’s, McNB. Accuracy = 80.3%, $\bar{A} = 65.3\%$, MCC = 0.794 CEN = 0.136.

McNB w/ Feature Selection This optimizer performs comparably to the baseline, being slightly better in MCC (0.794), CEN(0.136) and Accuracy(80.3%), but coming in slightly under in \bar{A} at 65.3%.

Hunter Due to numerous troubles getting the Hunters to run on this dataset, we still don’t have results from more than a few dozen generations. To be added as we get them. Our 1,925 generation run, which took 3 weeks, resulted in an MCC of 0.196, and a CEN of 0.307, which is better than random. However, because the training set was missing a handful of the more rare classes, it isn’t an apples-to-apples comparison.

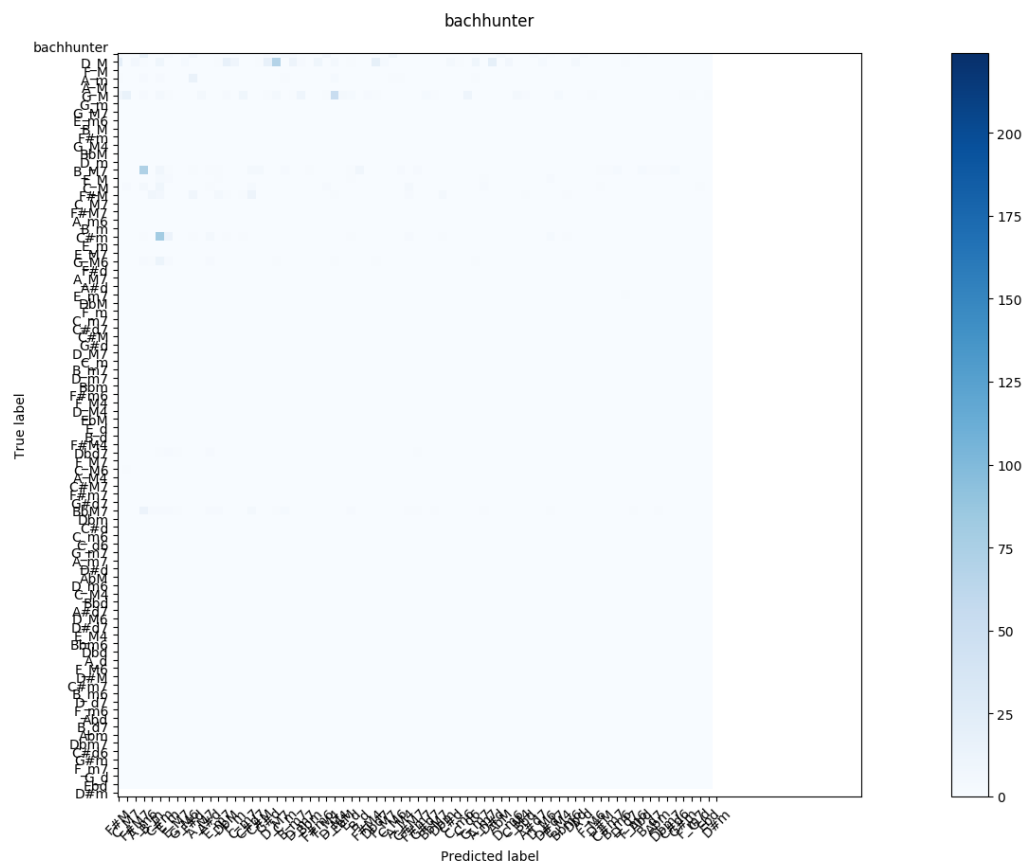


Figure 3.9: Bach's, Hunter. $MCC = 0.196$ $CEN = 0.307$.

3.3 Final Thoughts

It is clear that theoretically based algorithms are better at solving problems than trying to co-opt a GA to do it on its own. As for whether we should use McNB or CTree, the answer is clear: neither. We’ve already written far better performing algorithms elsewhere, including aggregate trees and support vector machine optimizers. The purpose of those algorithms was to give Hunters competition that wouldn’t completely outclass them, and they failed in that regard. This is at least partially because Naïve Bayes is such a robust first pass, and there are good reasons to use it in ensemble methods because it does such a good job extracting signal from messy data. Further, it does a decent job differentiating classes with few samples.

The most surprising performance was from CTree; while we have used trees in aggregate before, they performed far better alone than expected, in some regards holding their own up against Naïve Bayes, though mostly in terms of overall accuracy and only if we’re being accommodating. Still, their performance was better than we would have expected going into the project.

Hunters performed poorly. There might be some way of improving their performance, which we’ve noted as we’ve gone through the document. However, there should be a case made that such an endeavor is worthwhile, and one would need significant data contradicting this paper to say that there remains a compelling reason to do so. When we began this project, we believed that they had a decent chance to at least hold their own with our methods. This has been proven to be false across numerous comparisons. Further, we “cheated” on behalf of the Hunter, giving it vast additional resources, time, and modified starting conditions. We gave it every advantage, and it failed to deliver. The evidence is not conclusive for genetic algorithms in general, but this GA specifically is vastly inferior to even modest hybrid classification methods and should be retired.

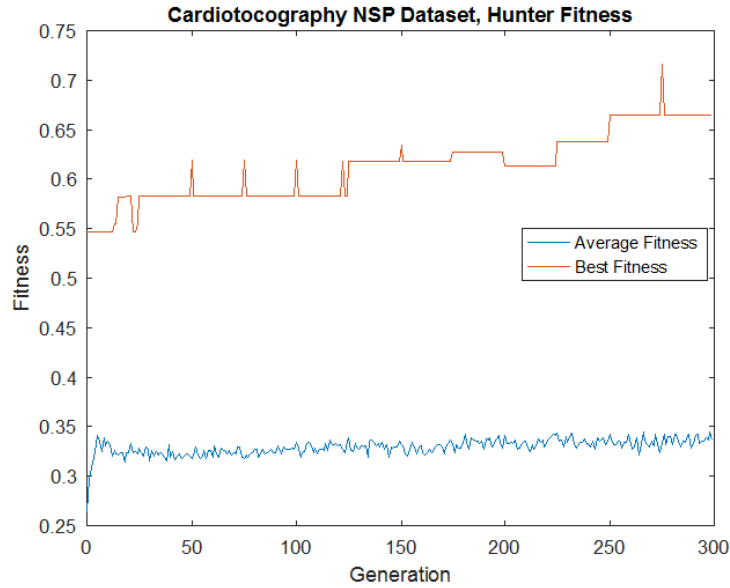


Figure 3.10: This figure demonstrates Hunter fitness, average and best, over the lifespan of a trial, in this case 300 generations. Where there seems to be lacking monotonicity is actually the result of validation fitness, which has the best Hunters seemingly scoring much better on the testing set.

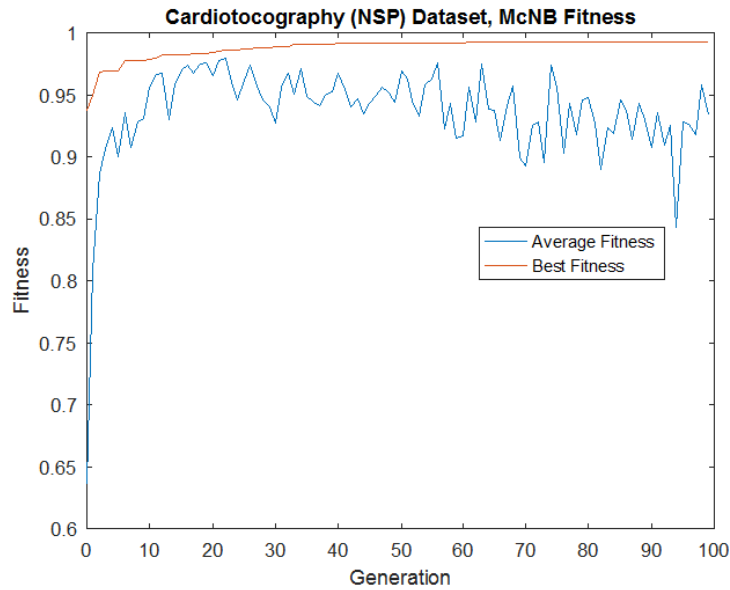


Figure 3.11: Population fitness of the McNB Optimizer on the CardioNSP dataset. This overall shape is typical of most Optimizers.

Chapter 4

Conclusions

Genetic Algorithms should probably be used to optimize rather than classify. Without considerably more work developing a better algorithm to create an extensible generic universal genetic classifier, there's simply too much theoretical ground to make up. GAs still do a good job optimizing, and can get the same or better performance out of them, which is very similar to the real evolution. This project felt like forcing a speedboat to race against kittens piloting a bucket, and then being shocked as even without any other advantages the speedboat won every time.

In the end, evolutionary algorithms are a swiss-army knife. Certainly, a GA would be able to solve linear programming problems better than a support vector machine, but that isn't even in the realm of a fair comparison. GAs are good at what they do, that is, optimizing a fitness function over time in a way that resembles evolution. They can easily be overwhelmed with genomes of great length, which is one area where real evolution has a huge edge. First, it is massively and embarrassingly parallel. Second, developmental biology is great at branch and bound. In other words, genomes that will have trouble producing viable solutions will themselves be less likely to exist because of many pass or fail tests along the way. Oh, and it also has a billion years or more to come up with solutions. If there were a way for GAs to take advantage of additional parallelism or checkpoints that might be

a place for further research. Another place might be in finding similarly generic tools which we could leverage, like, perhaps, neural nets to take a first pass at a dataset and then using a Hunter-like approach to distinguish results, though, if neural nets are already involved, there would need to be a good reason to invoke a Hunter when some other neural net would likely get better results, especially given their lackluster performance here. One possible reason for using Hunters despite their mediocre performance: they are extremely transparent. A Hunter will distill its decision making into unambiguous rules (even if it is a slew of them), where a neural net by its nature relies on numerous hidden calculations. This transparency was a major motivating factor for this approach to begin with.

Some other direction that might be worth pursuing is finding a way to combine more theoretical underpinnings with a GA. For instance, here the mechanics available to the Hunter were somewhat lackluster. All they could do were make boolean decisions based on the absolute values of features. That's simply not enough for modern datasets. As mentioned, GAs are extremely good at leveraging tools given to them and combining them in interesting ways, so one might consider improving the quality of the toolbox a useful avenue for further research. This could be branching on any number of concepts, including statistical ones or neural network inspired, or perhaps abandoning ensemble voting altogether and coming to some conclusion more akin to maximum likelihood estimation. An example of that might be building different PDFs for each class from an arbitrary number of Gaussian functions and evaluating based on the resulting metrics.

\overline{A} has proved to be a flawed metric, as to some degree all metrics are. We would still argue that it is less flawed than anything simpler. Until this result, our findings with \overline{A} is that it was usually \approx to accuracy. Here, however, whether because of the skew of the datasets or some other confounding factor, \overline{A} was often very different from raw accuracy, which is a place for either further research or a reason to find a new metric. In hindsight, and even from an *a priori* standpoint, it seems obvious that if you only consider the diagonal of a confusion matrix you're losing useful information. [Jurman](#)

et al. (2012) includes a few methods which might be valuable for multi-class confusion matrices. Matthew's Correlation Coefficient and Confusion Entropy seem promising, and implementing them as a fitness function would be fairly straightforward. We calculate these metrics for the classifications we have already gathered, however future work might include using one or a weighted combination of both as better metrics for scoring multi-class classifiers.

The optimizers performed well, given relatively very few generations. The next area of research for them is combining them and connecting their outputs back into another optimizer for a difficult or intractable dataset, combining them in novel ways to get the maximum signal from a dataset, perhaps even a meta-optimizer that will optimize an ensemble of disparate optimizers, themselves optimizing primitive classifiers. That seems like a promising way of limiting the search length for each population of optimizers while still searching a much larger space, though more research would be needed to show that it is viable. For instance, the meta-optimizer could have a few bits for each subordinate optimizer, probably of different types. The first section of the bits would encode two numbers, the first for how many optimizers to train and the second for how many features to include. Then, the subordinate optimizers would operate under the constraint of including no more than the number of features, and would separately and quickly evolve an ensemble of different classifiers. These classifiers in turn would provide their output to the meta-optimizer who would then optimize a classifier of its own using all the features and the classifications made by its ensemble of classifiers as a new table. This might be feasible given the speed with which many of the classifiers were able to evolve, and the robustness of the classifiers generated in such a manner.

Bibliography

Bibliography

- Affenzeller, M. and Wagner, S. (2003). A self-adaptive model for selective pressure handling within the theory of genetic algorithms. In *International Conference on Computer Aided Systems Theory*, pages 384–393. Springer. [4](#)
- Alexandre, E., Cuadra, L., Salcedo-Sanz, S., Pastor-Sánchez, A., and Casanova-Mateo, C. (2015). Hybridizing Extreme Learning Machines and Genetic Algorithms to select acoustic features in vehicle classification applications. *Neurocomputing*, 152:58–68. [15](#)
- Ayres-de campos, D., Bernardes, J., Garrido, A., Marques-de s, J., and Pereira-leite, L. (2000). SisPorto 2.0: A Program for Automated Analysis of Cardiotocograms. *Journal of Maternal-Fetal Medicine*, 9(5):311–318. [49](#)
- Back, T. (1994). Selective pressure in evolutionary algorithms: a characterization of selection mechanisms. In *Proceedings of the First IEEE Conference on Evolutionary Computation. IEEE World Congress on Computational Intelligence*, pages 57–62 vol.1. [4](#)
- CEDAR (2002). CEDAR Databases. [17](#)
- Chou, J.-S., Cheng, M.-Y., Wu, Y.-W., and Pham, A.-D. (2014). Optimizing parameters of support vector machine using fast messy genetic algorithm for dispute classification. *Expert Systems with Applications*, 41(8):3955–3964. [14](#)

- Daniele P. Radicioni and Roberto Esposito (2014). UCI Machine Learning Repository: Bach Choral Harmony Data Set. [13](#), [48](#)
- Dehuri, S., Patnaik, S., Ghosh, A., and Mall, R. (2008). Application of elitist multi-objective genetic algorithm for classification rule generation. *Applied Soft Computing*, 8(1):477–487. [15](#)
- Devos, O., Downey, G., and Duponchel, L. (2014). Simultaneous data pre-processing and SVM classification model selection based on a parallel genetic algorithm applied to spectroscopic data of olive oils. *Food Chemistry*, 148:124–130. [15](#)
- Duan, L., Guo, L., Liu, K., Liu, E. H., and Li, P. (2014). Characterization and classification of seven Citrus herbs by liquid chromatographyquadrupole time-of-flight mass spectrometry and genetic algorithm optimized support vector machines. *Journal of Chromatography A*, 1339:118–127. [14](#)
- Fidelis, M. V., Lopes, H. S., and Freitas, A. A. (2000). Discovering comprehensible classification rules with a genetic algorithm. In *Proceedings of the 2000 Congress on Evolutionary Computation. CEC00 (Cat. No.00TH8512)*, volume 1, pages 805–810 vol.1. [16](#)
- Hoque, M. S., Mukit, M. A., and Bikas, M. A. N. (2012). An Implementation of Intrusion Detection System Using Genetic Algorithm. *International Journal of Network Security & Its Applications*, 4(2):109–120. arXiv: 1204.1336. [16](#)
- Hyafil, L. and Rivest, R. L. (1976). Constructing optimal binary decision trees is NP-complete. *Information processing letters*, 5(1):15–17. [27](#)
- J. P. Marques de S, J. Bernardes, and D. Ayres de Campos (2010). UCI Machine Learning Repository: Cardiotocography Data Set. [13](#), [48](#)
- Jurman, G., Riccadonna, S., and Furlanello, C. (2012). A Comparison of MCC and CEN Error Measures in Multi-Class Prediction. *PLOS ONE*, 7(8):e41882. [46](#), [69](#)

- Kharm, N., Kowaliw, T., Clement, E., Jensen, C., Youssef, A., and Yao, J. (2004). PROJECT CellNet: EVOLVING AN AUTONOMOUS PATTERN RECOGNIZER. *International Journal of Pattern Recognition and Artificial Intelligence*, 18(06):1039–1056. [14](#), [17](#), [33](#), [36](#), [39](#)
- Kowaliw, T., Kharm, N., Jensen, C., Moghnieh, H., and Yao, J. (2004). CellNet Co-Ev: Evolving Better Pattern Recognizers Using Competitive Co-evolution. In *Genetic and Evolutionary Computation GECCO 2004*, pages 1090–1101. Springer, Berlin, Heidelberg. DOI: 10.1007/978-3-540-24855-2_119. [17](#)
- Kozeny, V. (2015). Genetic algorithms for credit scoring: Alternative fitness function performance comparison. *Expert Systems with Applications*, 42(6):2998–3004. [16](#)
- Li, L., Zhang, G., Nie, J., Niu, Y., and Yao, A. (2012). The Application of Genetic Algorithm to Intrusion Detection in MP2p Network. In *Advances in Swarm Intelligence*, pages 390–397. Springer, Berlin, Heidelberg. DOI: 10.1007/978-3-642-30976-2_47. [16](#)
- Lichman, M. (2013). *UCI Machine Learning Repository*. University of California, Irvine, School of Information and Computer Sciences. [13](#), [47](#)
- Maaten, L. v. d. and Hinton, G. (2008). Visualizing Data using t-SNE. *Journal of Machine Learning Research*, 9(Nov):2579–2605. [48](#)
- Marchetti, M., Onorati, F., Matteucci, M., Mainardi, L., Piccione, F., Silvoni, S., and Priftis, K. (2013). Improving the Efficacy of ERP-Based BCIs Using Different Modalities of Covert Visuospatial Attention and a Genetic Algorithm-Based Classifier. *PLOS ONE*, 8(1):e53946. [14](#)
- Nakai, K. and Kanehisa, M. (1992). A knowledge base for predicting protein localization sites in eukaryotic cells. *Genomics*, 14(4):897–911. [48](#)

- Ocak, H. (2013). A Medical Decision Support System Based on Support Vector Machines and the Genetic Algorithm for the Evaluation of Fetal Well-Being. *Journal of Medical Systems*, 37(2):9913. [14](#), [49](#)
- Paul Horton (1996). UCI Machine Learning Repository: Yeast Data Set. [13](#), [47](#)
- Radicioni, D. P. and Esposito, R. (2010). BREVE: An HMPerceptron-Based Chord Recognition System. In Ra, Z. W. and Wierzchowska, A. A., editors, *Advances in Music Information Retrieval*, number 274 in Studies in Computational Intelligence, pages 143–164. Springer Berlin Heidelberg. DOI: 10.1007/978-3-642-11674-2_7. [50](#)
- Ruiz, E., Albareda-Sambola, M., Fernndez, E., and Resende, M. G. C. (2015). A biased random-key genetic algorithm for the capacitated minimum spanning tree problem. *Computers & Operations Research*, 57:95–108. [4](#), [32](#)
- Salari, N., Shohaimi, S., Najafi, F., Nallappan, M., and Karishnarajah, I. (2014). A Novel Hybrid Classification Model of Genetic Algorithms, Modified k-Nearest Neighbor and Developed Backpropagation Neural Network. *PLOS ONE*, 9(11):e112987. [15](#)
- Schuman, C. D., Birdwell, J. D., and Dean, M. E. (2014). Spatiotemporal classification using neuroscience-inspired dynamic architectures. *Procedia Computer Science*, 41:89–97. [14](#)
- Srikanth, R., George, R., Warsi, N., Prabhu, D., Petry, F. E., and Buckles, B. P. (1995). A variable-length genetic algorithm for clustering and classification. *Pattern Recognition Letters*, 16(8):789–800. [16](#)
- Stefanie Scheid (2004). Introduction to Kernel Smoothing | Kernel (Operating System) | Probability Density Function. [25](#)
- Tseng, M.-H., Chen, S.-J., Hwang, G.-H., and Shen, M.-Y. (2008). A genetic algorithm rule-based approach for land-cover classification. *ISPRS Journal of Photogrammetry and Remote Sensing*, 63(2):202–212. [16](#)

- Uysal, A. K. and Gunal, S. (2014). Text classification using genetic algorithm oriented latent semantic features. *Expert Systems with Applications*, 41(13):5938–5947. [15](#)
- Wei, J.-M., Yuan, X.-J., Hu, Q.-H., and Wang, S.-Q. (2010). A novel measure for evaluating classifiers. *Expert Systems with Applications*, 37(5):3799–3809. [46](#)
- Wu, J., Long, J., and Liu, M. (2015). Evolving RBF neural networks for rainfall prediction using hybrid particle swarm optimization and genetic algorithm. *Neurocomputing*, 148:136–142. [14](#)
- Zhang, J. (2003). Evolution by gene duplication: an update. *Trends in Ecology & Evolution*, 18(6):292–298. [34](#)
- Zhang, Z., McDonnell, K. T., Zadok, E., and Mueller, K. (2015). Visual Correlation Analysis of Numerical and Categorical Data on the Correlation Map. *IEEE Transactions on Visualization and Computer Graphics*, 21(2):289–303. [21](#)

Appendix

Appendix A

Hunter Genomes and Explanations

A.1 Yeast

Aff	Cla	Not	Cell 1	Cell 2
01	0111	1	100000000110010111011	
11	0101	1	111011011100111100001	
11	0001	0	010001100101111101011	
10	0011	1	001001100110111010100	
11	0000	1	110110101001110001001	
10	0010	1	001101100010111101110	
11	0101	1	000000101001110111000	110100101110001110100
00	0110	0	101001101001111001101	011000001011011101010
11	0100	1	000000011000101010111	
11	1000	1	000010101001110110011	
11	0001	0	011101101011111010011	

cont'd

Aff	Cla	Not	Cell 1	Cell 2
10	1000	0	010101011011101011101	110010011111101111101
01	1001	0	100000101110100110111	
00	0000	0	001101011000110010110	
01	1001	1	000100111111101101111	
11	0001	1	001100011001101010100	
01	0111	0	000100001000010010110	
11	0101	0	100000110011101111101	
01	0100	0	011110110001111111001	
10	0011	1	000100110000101101001	
01	0011	0	011101011101110101010	
11	0100	1	111001100000110101010	
01	0001	0	011101011001110000101	
01	0111	1	011001100101110111001	

A.1: Best Hunter, Yeast

```
1 This hunter has the following 24 chromosomes:
2 This chromosome prefers the rear
3 It focuses on problems in the following class:
4 VAC
5 By aggregating the nay votes from the following 1 cell:
6 This cell looks at feature 0
7 whose return value is between 0.0234375 and 0.36328125
8
9 This chromosome considers itself complete
10 It focuses on problems in the following class:
11 ME2
12 By aggregating the nay votes from the following 1 cell:
13 This cell looks at feature 6
14 whose return value is between 0.859375 and 0.9375
15
16 This chromosome considers itself complete
17 It focuses on problems in the following class:
18 NUC
19 By aggregating the yes votes from the following 1 cell:
20 This cell looks at feature 4
21 whose return value is not between 0.39453125 and 0.95703125
22
23 This chromosome prefers the front
24 It focuses on problems in the following class:
25 ME1
26 By aggregating the nay votes from the following 1 cell:
27 This cell looks at feature 2
28 whose return value is not between 0.3984375 and 0.9140625
29
```

30 This chromosome considers itself complete
 31 It focuses on problems in the following class:
 32 MIT
 33 By aggregating the nay votes from the following 1 cell:
 34 This cell looks at feature 5
 35 whose return value is between 0.66015625 and 0.765625
 36
 37 This chromosome prefers the front
 38 It focuses on problems in the following class:
 39 CYT
 40 By aggregating the nay votes from the following 1 cell:
 41 This cell looks at feature 3
 42 whose return value is not between 0.3828125 and 0.96484375
 43
 44 This chromosome considers itself complete
 45 It focuses on problems in the following class:
 46 ME2
 47 By aggregating the nay votes from the following 2 cells:
 48 This cell looks at feature 0
 49 whose return value is not between 0.16015625 and 0.859375
 50
 51 This cell looks at feature 5
 52 whose return value is between 0.1796875 and 0.2265625
 53
 54 This chromosome has no preference
 55 It focuses on problems in the following class:
 56 ME3
 57 By aggregating the yes votes from the following 2 cells:
 58 This cell looks at feature 2
 59 whose return value is between 0.41015625 and 0.8984375

60
61 This cell looks at feature 6
62 whose return value is not between 0.04296875 and 0.45703125
63
64 This chromosome considers itself complete
65 It focuses on problems in the following class:
66 EXC
67 By aggregating the nay votes from the following 1 cell:
68 This cell looks at feature 0
69 whose return value is not between 0.09375 and 0.66796875
70
71 This chromosome considers itself complete
72 It focuses on problems in the following class:
73 POX
74 By aggregating the nay votes from the following 1 cell:
75 This cell looks at feature 0
76 whose return value is not between 0.66015625 and 0.84765625
77
78 This chromosome considers itself complete
79 It focuses on problems in the following class:
80 NUC
81 By aggregating the yes votes from the following 1 cell:
82 This cell looks at feature 7
83 whose return value is not between 0.41796875 and 0.91015625
84
85 This chromosome prefers the front
86 It focuses on problems in the following class:
87 POX
88 By aggregating the yes votes from the following 2 cells:
89 This cell looks at feature 5

90 whose return value is not between 0.35546875 and 0.6796875
 91
 92 This cell looks at feature 4
 93 whose return value is between 0.62109375 and 0.7421875
 94
 95 This chromosome prefers the rear
 96 It focuses on problems in the following class:
 97 ERL
 98 By aggregating the yes votes from the following 1 cell:
 99 This cell looks at feature 0
 100 whose return value is between 0.1796875 and 0.60546875
 101
 102 This chromosome has no preference
 103 It focuses on problems in the following class:
 104 MIT
 105 By aggregating the yes votes from the following 1 cell:
 106 This cell looks at feature 3
 107 whose return value is not between 0.34375 and 0.79296875
 108
 109 This chromosome prefers the rear
 110 It focuses on problems in the following class:
 111 ERL
 112 By aggregating the nay votes from the following 1 cell:
 113 This cell looks at feature 1
 114 whose return value is not between 0.24609375 and 0.71484375
 115
 116 This chromosome considers itself complete
 117 It focuses on problems in the following class:
 118 NUC
 119 By aggregating the nay votes from the following 1 cell:

120 This cell looks at feature 3
121 whose return value is not between 0.09765625 and 0.6640625
122
123 This chromosome prefers the rear
124 It focuses on problems in the following class:
125 VAC
126 By aggregating the yes votes from the following 1 cell:
127 This cell looks at feature 1
128 whose return value is not between 0.03125 and 0.29296875
129
130 This chromosome considers itself complete
131 It focuses on problems in the following class:
132 ME2
133 By aggregating the yes votes from the following 1 cell:
134 This cell looks at feature 0
135 whose return value is between 0.19921875 and 0.7421875
136
137 This chromosome prefers the rear
138 It focuses on problems in the following class:
139 EXC
140 By aggregating the yes votes from the following 1 cell:
141 This cell looks at feature 7
142 whose return value is not between 0.69140625 and 0.984375
143
144 This chromosome prefers the front
145 It focuses on problems in the following class:
146 ME1
147 By aggregating the nay votes from the following 1 cell:
148 This cell looks at feature 1
149 whose return value is not between 0.1875 and 0.703125

150
151 This chromosome prefers the rear
152 It focuses on problems in the following class:
153 ME1
154 By aggregating the yes votes from the following 1 cell:
155 This cell looks at feature 7
156 whose return value is not between 0.36328125 and 0.83203125
157
158 This chromosome considers itself complete
159 It focuses on problems in the following class:
160 EXC
161 By aggregating the nay votes from the following 1 cell:
162 This cell looks at feature 6
163 whose return value is between 0.375 and 0.83203125
164
165 This chromosome prefers the rear
166 It focuses on problems in the following class:
167 NUC
168 By aggregating the yes votes from the following 1 cell:
169 This cell looks at feature 7
170 whose return value is not between 0.34765625 and 0.7578125
171
172 This chromosome prefers the rear
173 It focuses on problems in the following class:
174 VAC
175 By aggregating the nay votes from the following 1 cell:
176 This cell looks at feature 6
177 whose return value is not between 0.39453125 and 0.859375

Vita

Vita goes here...