

# A Parallel Architecture for Data Mining and Knowledge Discovery

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## Abstract

In this paper, we introduce a new machine learning theory based on multi-channel parallel adaptation for rule discovery. This theory is distinguished from the familiar parallel-distributed adaptation theory of neural networks in terms of channel-based convergence to the target rules. We show how to realize this theory in a learning system named CFRule. CFRule is a parallel weight-based model, but it departs from traditional neural computing in that its internal knowledge is comprehensible. Furthermore, when the model converges upon training, each channel converges to a target rule. The model adaptation rule is derived by multi-level parallel weight optimization based on gradient descent. Since, however, gradient descent only guarantees local optimization, a multi-channel regression-based optimization strategy is developed to effectively deal with this problem. Formally, we prove that the CFRule model can explicitly and precisely encode any given rule set. Also, we prove a property related to asynchronous parallel convergence, which is a critical element of the multi-channel parallel adaptation theory for rule learning. Thanks to the quantizability nature of the CFRule model, rules can be extracted completely and soundly via a threshold-based mechanism. Finally, the practical application of the theory is demonstrated in DNA promoter recognition and hepatitis prognosis prediction.

**Keywords:** rule discovery, adaptation, optimization, regression, certainty factor, neural network, machine learning, uncertainty management, artificial intelligence.

## 1 Introduction

Rules express general knowledge about actions or conclusions in given circumstances and also principles in given domains. In the if-then format, rules are an easy way to represent cognitive processes in psychology and a useful means to encode expert knowledge. In another perspective, rules are important because they can help scientists understand problems and engineers solve problems. These observations would account for the fact that rule learning or discovery has become a major topic in both machine learning and data mining research. The former discipline concerns the construction of computer programs which learn knowledge or skill while the latter is about the discovery of patterns or rules hidden in the data.

The fundamental concepts of rule learning are discussed in [16]. Methods for learning sets of rules include symbolic heuristic search [3, 5], decision trees [17-18], inductive logic programming [13], neural networks [2, 7, 20], and genetic algorithms [10]. A methodology comparison can be found

in our previous work [9]. Despite the differences in their computational frameworks, these methods perform a certain kind of search in the rule space (i.e., the space of possible rules) in conjunction with some optimization criterion. Complete search is difficult unless the domain is small, and a computer scientist is not interested in exhaustive search due to its exponential computational complexity. It is clear that significant issues have limited the effectiveness of all the approaches described. In particular, we should point out that all the algorithms except exhaustive search guarantee only local but not global optimization. For example, a sequential covering algorithm such as CN2 [5] performs a greedy search for a single rule at each sequential stage without backtracking and could make a suboptimal choice at any stage; a simultaneous covering algorithm such as ID3 [18] learns the entire set of rules simultaneously but it searches incompletely through the hypothesis space because of attribute ordering; a neural network algorithm which adopts gradient-descent search is prone to local minima.

In this paper, we introduce a new machine learning theory based on multi-channel parallel adaptation that shows great promise in learning the target rules from data by parallel global convergence. This theory is distinct from the familiar parallel-distributed adaptation theory of neural networks in terms of channel-based convergence to the target rules. We describe a system named CFRule which implements this theory. CFRule bases its computational characteristics on the certain factor (CF) model [4, 22] it adopts. The CF model is a calculus of uncertainty management and has been used to approximate standard probability theory [1] in artificial intelligence. It has been found that certainty factors associated with rules can be revised by a neural network [6, 12, 15]. Our research has further indicated that the CF model used as the neuron activation function (for combining inputs) can improve the neural-network performance [8].

The rest of the paper is organized as follows. Section 2 describes the multi-channel rule learning model. Section 3 examines the formal properties of rule encoding. Section 4 derives the model parameter adaptation rule, presents a novel optimization strategy to deal with the local minimum problem due to gradient descent, and proves a property related to asynchronous parallel convergence, which is a critical element of the main theory. Section 5 formulates a rule extraction algorithm. Section 6 demonstrates practical applications. Then we draw conclusions in the final section.

## 2 The Multi-Channel Rule Learning Model

CFRule is a rule-learning system based on multi-level parameter optimization. The kernel of CFRule is a multi-channel rule learning model. CFRule can be embodied as an artificial neural network, but the neural network structure is not essential. We start with formal definitions about the model.

**Definition 2.1** *The multi-channel rule learning model  $M$  is defined by  $k$  ( $k \geq 1$ ) channels ( $Ch$ 's), an input vector ( $M_{in}$ ), and an output ( $M_{out}$ ) as follows:*

$$M \equiv (Ch_1, Ch_2, \dots, Ch_k, M_{in}, M_{out}) \quad (1)$$

where  $-1 \leq M_{out} \leq 1$  and

$$M_{in} \equiv (x_1, x_2, \dots, x_d) \quad (2)$$

such that  $d$  is the input dimensionality and  $-1 \leq x_i \leq 1$  for all  $i$ .

The model has only a single output because here we assume the problem is a single-class, multi-rule learning problem. The framework can be easily extended to the multi-class case.

**Definition 2.2** *Each channel ( $Ch_j$ ) is defined by an output weight ( $u_j$ ), a set of input weights ( $w_{ji}$ 's), activation ( $\phi_j$ ), and influence ( $\psi_j$ ) as follows:*

$$Ch_j \equiv (u_j, w_{j0}, w_{j1}, w_{j2}, \dots, w_{jd}, \phi_j, \psi_j) \quad (3)$$

where  $w_{j0}$  is the bias,  $0 \leq u_j \leq 1$ , and  $-1 \leq w_{ji} \leq 1$  for all  $i$ . The input weight vector ( $w_{j1}, \dots, w_{jd}$ ) defines the channel's pattern.

**Definition 2.3** *Each channel's activation is defined by*

$$\phi_j = f_{cf}(w_{j0}, w_{j1}x_1, w_{j2}x_2, \dots, w_{jd}x_d) \quad (4)$$

where  $f_{cf}$  is the CF-combining function [4, 22], as defined below.

**Definition 2.4** *The CF-combining function is given by*

$$f_{cf}(x_1, x_2, \dots, y_1, y_2, \dots) = f_{cf}^+(x_1, x_2, \dots) + f_{cf}^-(y_1, y_2, \dots) \quad (5)$$

where

$$f_{cf}^+(x_1, x_2, \dots) = 1 - \prod_i (1 - x_i) \quad (6)$$

$$f_{cf}^-(y_1, y_2, \dots) = -1 + \prod_j (1 + y_j) \quad (7)$$

$x_i$ 's are nonnegative numbers and  $y_j$ 's are negative numbers.

As we will see, the CF-combining function contributes to several important computational properties instrumental to rule discovery.

**Definition 2.5** *Each channel's influence on the output is defined by*

$$\psi_j = u_j \phi_j \quad (8)$$

**Definition 2.6** *The model output  $M_{out}$  is defined by*

$$M_{out} = f_{cf}(\psi_1, \psi_2, \dots, \psi_k) \quad (9)$$

We call the class whose rules to be learned the *target class*, and define rules inferring (or explaining) that class to be the *target rules*. For instance, if the disease diabetes is the target class, then the diagnostic rules for diabetes would be the target rules. Each target rule defines a condition under which the given class can be inferred. Note that we do not consider rules which deny the target class, though such rules can be defined by reversing the class concept. The task of rule learning is to learn or discover a set of target rules from given instances called training instances (data). It is important that rules learned should be generally applicable to the entire domain, not just the training data. How well the target rules learned from the training data can be applied to unseen data determines the generalization performance.

Instances which belong to the target class are called positive instances, else, called negative instances. Ideally, a positive training instance should match at least one target rule learned and vice versa, whereas a negative training instance should match none. So, if there is only a single target rule learned, then it must be matched by all (or most) positive training instances. But if multiple target rules are learned, then each rule is matched by some (rather than all) positive training instances. Since the number of possible rule sets is far greater than the number of possible rules, the problem of learning multiple rules is naturally much more complex than that of learning single rules.

In the multi-channel rule learning theory, the model learns to sort out instances so that instances belonging to different rules flow through different channels, and at the same time, channels are adapted to accommodate their pertinent instances and learn corresponding rules. Notice that this is a mutual process and it cannot occur all at once. In the beginning, the rules are not learned and the channels are not properly shaped, both information flow and adaptation are more or less random, but through self-adaptation, the CFRule model will gradually converge to the correct rules, each encoded by a channel. The essence of this paper is to prove this property.

In the model design, a legitimate question is what the optimal number of channels is. This is just like the question raised for a neural network of how many hidden (internal computing) units should be used. It is true that too many hidden units cause data overfitting and make generalization worse [7]. Thus, a general principle is to use a minimal number of hidden units. The same principle can be equally well applied to the CFRule model. However, there is a difference. In ordinary neural networks, the number of hidden units is determined by the sample size, while in the CFRule model, the number of channels should match the number of rules embedded in the data. Since, however, we do not know how many rules are present in the data, our strategy is to use a minimal number of channels that admits convergence on the training data.

The model's behavior is characterized by three aspects:

- Information processing: Compute the model output for a given input vector.
- Learning or training: Adjust channels’ parameters (output and input weights) so that the input vector is mapped into the output for every instance in the training data.
- Rule extraction: Extract rules from a trained model.

The first aspect has been described already.

### 3 Model Representation of Rules

The IF-THEN rule (i.e., If the premise, then the action) is a major knowledge representation paradigm in artificial intelligence. Here we make analysis of how such rules can be represented with proper semantics in the CFRule model.

**Definition 3.1** *CFRule learns rules in the form of*

*IF  $A_1^+, \dots, A_i^+, \dots, \neg A_1^-, \dots, \neg A_j^-, \dots$ , THEN the target class with a certainty factor.*

where  $A_i^+$  is a positive antecedent (in the positive form),  $A_j^-$  a negated antecedent (in the negative form), and  $\neg$  reads “not.” Each antecedent can be a discrete or discretized attribute (feature), variable, or a logic proposition. The IF part must not be empty. The attached certainty factor in the THEN part, called the rule CF, is a positive real  $\leq 1$ .

The rule’s premise is restricted to a conjunction, and no disjunction is allowed. The collection of rules for a certain class can be formulated as a DNF (disjunctive normal form) logic expression, namely, the disjunction of conjunctions, which implies the class. However, rules defined here are not traditional logic rules because of the attached rule CFs meant to capture uncertainty. We interpret a rule by saying when its premise holds (that is, all positive antecedents mentioned are true and all negated antecedents mentioned are false), the target concept holds at the given confidence level. CFRule can also learn rules with weighted antecedents (a kind of fuzzy rules), but we will not consider this case here.

There is increasing evidence to indicate that good rule encoding capability actually facilitates rule discovery in the data. In the theorems that follow, we show how the CFRule model can explicitly and precisely encode any given rule set. We note that the ordinary sigmoid-function neural network can only implicitly and approximately do this. Also, we note although the threshold function of the perceptron model enables it to learn conjunctions or disjunctions, the non-differentiability of this function prohibits the use of an adaptive procedure in a multilayer construct.

**Theorem 3.1** *For any rule represented by Definition 3.1, there exists a channel in the CFRule model to encode the rule so that if an instance matches the rule, the channel’s activation is 1, else 0.*

(Proof): This can be proven by construction. Suppose we implement channel  $j$  by setting the bias weight to 1, the input weights associated with all positive attributes in the rule’s premise to 1, the input weights associated with all negated attributes in the rule’s premise to  $-1$ , the rest of the input weights to 0, and finally the output weight to the rule CF. Assume that each instance is encoded by a bipolar vector in which for each attribute, 1 means true and  $-1$  false. When an instance matches the rule, the following conditions hold:  $x_i = 1$  if  $x_i$  is part of the rule’s premise,  $x_i = -1$  if  $\neg x_i$  is part of the rule’s premise, and otherwise  $x_i$  can be of any value. For such an instance, given the above construction, it is true that  $w_{ji}x_i = 1$  or 0 for all  $i$ . Thus, the channel’s activation (by Definition 2.3),

$$\phi_j = f_{cf}(w_{j0} = 1, w_{j1}x_1, w_{j2}x_2, \dots, w_{jd}x_d) \quad (10)$$

must be 1 according to  $f_{cf}$ . On the other hand, if an instance does not match the rule, then there exists  $i$  such that  $w_{ji}x_i = -1$ . Since  $w_{j0}$  (the bias weight) = 1, the channel’s activation is 0 due to  $f_{cf}$ .  $\square$

**Theorem 3.2** *Assume that rule CF’s  $> \theta$  ( $0 \leq \theta \leq 1$ ). For any set of rules represented by Definition 3.1, there exists a CFRule model to encode the rule set so that if an instance matches any of the given rules, the model output is  $> \theta$ , else 0.*

(Proof): Suppose there are  $k$  rules in the set. As suggested in the proof of Theorem 3.1, we construct  $k$  channels, each encoding a different rule in the given rule set so that if an instance matches, say rule  $j$ , then the activation ( $\phi_j$ ) of channel  $j$  is 1. In this case, since the channel’s influence  $\psi_j$  is given by  $u_j\phi_j$  (where  $u_j$  is set to the rule CF) and the rule CF  $> \theta$ , it follows that  $\psi_j > \theta$ . It is then clear that the model output must be  $> \theta$  since it combines influences from all channels that  $\geq 0$  but at least one  $> \theta$ . On the other hand, if an instance fails to match any of the rules, all the channels’ activations are zero, so is the model output.  $\square$

## 4 Model Adaptation and Convergence

In neural computing, the backpropagation algorithm [19] can be viewed as a multilayer, parallel optimization strategy that enables the network to converge to a local optimum solution. The black-box nature of the neural network solution is reflected by the fact that the pattern (the input weight vector) learned by each neuron does not bear meaningful knowledge. The CFRule model departs from traditional neural computing in that its internal knowledge is comprehensible. Furthermore, when the model converges upon training, each channel converges to a target rule. How to achieve this objective and what is the mathematical theory are the main issues to be addressed.

### 4.1 Model Training Based on Gradient Descent

The CFRule model learns to map a set of input vectors (e.g., extracted features) into a set of outputs (e.g., class

information) by training. An input vector along with its target output constitute a training instance. The input vector is encoded as a  $1/-1$  bipolar vector. The target output is 1 for a positive instance and 0 for a negative instance.

Starting with a random or estimated weight setting, the model is trained to adapt itself to the characteristics of the training instances by changing weights (both output and input weights) for every channel in the model. Typically, instances are presented to the model one at a time. When all instances are examined (called an epoch), the network will start over with the first instance and repeat. Iterations continue until the system performance has reached a satisfactory level.

The learning rule of the CFRule model is derived in the same way as the backpropagation algorithm [19]. The training objective is to minimize the sum of squared errors in the data. In each learning cycle, a training instance is given and the weights of channel  $j$  (for all  $j$ ) are updated by

$$u_j(t+1) = u_j(t) + \Delta u_j \quad (11)$$

$$w_{ji}(t+1) = w_{ji}(t) + \Delta w_{ji} \quad (12)$$

where  $u_j$ : the output weight,  $w_{ji}$ : an input weight, the argument  $t$  denotes iteration  $t$ , and  $\Delta$  the adjustment. The weight adjustment on the current instance is based on gradient descent. Consider channel  $j$ . For the output weight ( $u_j$ ),

$$\Delta u_j = -\eta(\partial E/\partial u_j) \quad (13)$$

( $\eta$ : the learning rate) where

$$E = \frac{1}{2}(T_{out} - M_{out})^2$$

( $T_{out}$ : the target output,  $M_{out}$ : the model output). Let

$$D = T_{out} - M_{out}$$

The partial derivative in Eq. (13) can be rewritten with the calculus chain rule to yield

$$\partial E/\partial u_j = (\partial E/\partial M_{out})(\partial M_{out}/\partial u_j) = -D(\partial M_{out}/\partial u_j)$$

Then we apply this result to Eq. (13) and obtain the following definition.

**Definition 4.1** *The learning rule for output weight  $u_j$  of channel  $j$  is given by*

$$\Delta u_j = \eta D(\partial M_{out}/\partial u_j) \quad (14)$$

For the input weights ( $w_{ji}$ 's), again based on gradient descent,

$$\Delta w_{ji} = -\eta(\partial E/\partial w_{ji}) \quad (15)$$

The partial derivative in Eq. (15) is equivalent to

$$\partial E/\partial w_{ji} = (\partial E/\partial \phi_j)(\partial \phi_j/\partial w_{ji})$$

Since  $\phi_j$  is not directly related to  $E$ , the first partial derivative on the right hand side of the above equation is expanded by the chain rule again to obtain

$$\partial E/\partial \phi_j = (\partial E/\partial M_{out})(\partial M_{out}/\partial \phi_j) = -D(\partial M_{out}/\partial \phi_j)$$

Substituting these results into Eq. (15) leads to the following definition.

**Definition 4.2** *The learning rule for input weight  $w_{ji}$  of channel  $j$  is given by*

$$\Delta w_{ji} = \eta d_j(\partial \phi_j/\partial w_{ji}) \quad (16)$$

where

$$d_j = D(\partial M_{out}/\partial \phi_j)$$

Assume that

$$\phi_j = f_{cf}^+(w_{j1}x_1, w_{j2}x_2, \dots, w_{jd'}x_{d'}) + f_{cf}^-(w_{jd'+1}x_{d'+1}, \dots, w_{jd}x_d) \quad (17)$$

Suppose  $d' > 1$  and  $d - d' > 1$ . The partial derivative  $\frac{\partial \phi_j}{\partial w_{ji}}$  can be computed as follows.

Case (a) If  $w_{ji}x_i \geq 0$ ,

$$\frac{\partial \phi_j}{\partial w_{ji}} = \left( \prod_{l \neq i, l \leq d'} (1 - w_{jl}x_l) \right) x_i \quad (18)$$

Case (b) If  $w_{ji}x_i < 0$ ,

$$\frac{\partial \phi_j}{\partial w_{ji}} = \left( \prod_{l \neq i, l > d'} (1 + w_{jl}x_l) \right) x_i \quad (19)$$

It is easy to show that if  $d' = 1$  in case (a) or  $d - d' = 1$  in case (b),  $\frac{\partial \phi_j}{\partial w_{ji}} = x_i$ .

## 4.2 Multi-Channel Regression-Based Optimization

It is known that gradient descent can only find a local minimum. When the error surface is flat or very convoluted, such an algorithm often ends up with a bad local minimum. Moreover, the learning performance is measured by the error on unseen data independent of the training set. Such error is referred to as generalization error. We note that minimization of the training error by the backpropagation algorithm does not guarantee simultaneous minimization of generalization error. What is worse, generalization error may instead rise after some point along the training curve due to an undesired phenomenon known as overfitting [7]. Thus, global optimization techniques for network training (e.g., [21]) do not necessarily offer help as far as generalization is concerned. To address this issue, CFRule uses a novel optimization strategy called multi-channel regression-based optimization (MCRO).

In Definition 2.4,  $f_{cf}^+$  and  $f_{cf}^-$  can also be expressed as

$$f_{cf}^+(x_1, x_2, \dots) = \sum_i x_i - \sum_i \sum_j x_i x_j + \sum_i \sum_j \sum_k x_i x_j x_k - \dots \quad (20)$$

$$f_{cf}^-(y_1, y_2, \dots) = \sum_i y_i + \sum_i \sum_j y_i y_j + \sum_i \sum_j \sum_k y_i y_j y_k + \dots \quad (21)$$

When the arguments ( $x_i$ 's and  $y_i$ 's) are small, the CF function behaves somewhat like a linear function. It can

be seen that if the magnitude of every argument is  $< 0.1$ , the first order approximation of the CF function is within an error of 10% or so. Since when learning starts, all the weights take on small values, this analysis has motivated the MCRO strategy for improving the gradient descent solution. The basic idea behind MCRO is to choose a starting point based on the linear regression analysis, in contrast to gradient descent which uses a random starting point.

If we can use regression analysis to estimate the initial influence of each input variable on the model output, how can we know how to distribute this estimate over multiple channels? In fact, this is the most intricate part of the whole idea since each channel's structure and parameters are yet to be learned. The answer will soon be clear.

In CFRule, each channel's activation is defined by

$$\phi_j = f_{cf}(w_{j0}, w_{j1}x_1, w_{j2}x_2, \dots) \quad (22)$$

Suppose we separate the linear component from the non-linear component ( $R$ ) in  $\phi_j$  to obtain

$$\phi_j = \left( \sum_{i=0}^d w_{ji}x_i \right) + R_j \quad (23)$$

We apply the same treatment to the model output (Definition 2.6)

$$M_{out} = f_{cf}(u_1\phi_1, u_2\phi_2, \dots) \quad (24)$$

so that

$$M_{out} = \left( \sum_{j=1}^k u_j\phi_j \right) + R_{out} \quad (25)$$

Then we substitute Eq.(23) into Eq.(25) to obtain

$$M_{out} = \left( \sum_{j=1}^k \sum_{i=0}^d u_j w_{ji} x_i \right) + R_{acc} \quad (26)$$

in which the right hand side is equivalent to

$$\left[ \sum_{i=0}^d \left( \sum_{j=1}^k u_j w_{ji} \right) x_i \right] + R_{acc}$$

Note that

$$R_{acc} = \left( \sum_{j=1}^k u_j R_j \right) + R_{out}$$

Suppose linear regression analysis produces the following estimation equation for the model output:

$$M'_{out} = b_0 + b_1 x_1 + \dots$$

(all the input variables and the output transformed to the range from 0 to 1).

**Definition 4.3** The MCRO strategy is defined by

$$\sum_{j=1}^k u_j(t=0)w_{ji}(t=0) = b_i \quad (27)$$

for each  $i, 0 \leq i \leq d$

Table 1: The target rules in the simulation experiment.

rule 1:	IF $x_1$ and $\neg x_2$ and $x_7$	THEN the target concept
rule 2:	IF $x_1$ and $\neg x_4$ and $x_5$	THEN the target concept
rule 3:	IF $x_6$ and $x_{11}$	THEN the target concept

That is, at iteration  $t = 0$  when learning starts, the initial weights are randomized but subject to these  $d + 1$  constraints.

To demonstrate this strategy, we designed an experiment. Assume there were 20 input variables and three targets rules as shown in Table 1. The training and test data sets were generated independently, each consisting of 100 random instances. An instance was classified as positive if it matched any of the target rules and as negative otherwise. The CFRule model for this experiment comprised three channels. The model was trained under MCRO and random start separately. For each strategy, 25 trials were run, each with a different initial weight setting. The same learning rate and stopping condition were used in every trial regardless of the strategy taken. The training and test error rates were measured. If the model converged to the target rules, then both training and test errors should be close to zero. We used the  $t$  test (one-sided hypothesis testing based on the statistical  $t$  distribution) to evaluate the difference in the means of error rates produced under the two strategies. Given the statistical validation result, we can conclude that MCRO is a valid technique.

### 4.3 Asynchronous Parallel Convergence

In the multi-channel rule learning theory, there are two possible modes of parallel convergence. In the synchronous mode, all channels converge to their respective target patterns at the same time, whereas in the asynchronous mode, each channel converges at a different time. In a self-adaptation or self-organization model without a global clock, the synchronous mode is not a plausible scenario of convergence. On the other hand, the asynchronous mode may not arrive at global convergence (i.e., every channel converging to its target pattern) unless there is a mechanism to protect a target pattern once it is converged upon. Here we examine a formal property of CFRule on this new learning issue.

**Theorem 4.1** Suppose at time  $t$ , channel  $j$  of the CFRule model has learned an exact pattern  $(w_{j1}, w_{j2}, \dots, w_{jd})$  ( $d \geq 1$ ) such that  $w_{j0}$  (the bias) = 1 and  $w_{ji} = 1$  or  $-1$  or 0 for  $1 \leq i \leq d$ . At time  $t + 1$  when the model is trained on a given instance with the input vector  $(x_0, x_1, x_2, \dots, x_d)$  ( $x_0 = 1$  and  $x_i = 1$  or  $-1$  for all  $1 \leq i \leq d$ ), the pattern is unchanged unless there is a single mismatched weight (weight  $w_{ji}$  is mismatched if and only if  $w_{ji}x_i = -1$ ). Let  $\Delta w_{ji}(t + 1)$  be the weight adjustment for  $w_{ji}$ . Then (a) If there is no mismatch, then  $\Delta w_{ji}(t + 1) = 0$  for all  $i$ .

(b) If there are more than one mismatched weight then  $\Delta w_{ji}(t+1) = 0$  for all  $i$ .

(Proof): In case (a), there is no mismatch, so  $w_{ji}x_i = 1$  or 0 for all  $i$ . There exists  $l$  such that  $w_{jl}x_l = 1$  and  $l \neq i$ , for example,  $w_{j0}x_0 = 1$  as given. From Eq. (18),

$$\frac{\partial \phi_j}{\partial w_{ji}} = \left( \prod_{l \geq 0, l \neq i}^d (1 - w_{jl}x_l) \right) x_i = 0$$

Then from Eq. (16),

$$\Delta w_{ji}(t+1) = \eta d_j \left( \frac{\partial \phi_j}{\partial w_{ji}} \right) = 0$$

In case (b), the proof for matched weights is the same as that in case (a). Consider only mismatched weights  $w_{ji}$ 's such that  $w_{ji}x_i = -1$ . Since there are at least two mismatched weights, there exists  $l$  such that  $w_{jl}x_l = -1$  and  $l \neq i$ . From Eq. (19),

$$\frac{\partial \phi_j}{\partial w_{ji}} = \left( \prod_{w_{jl}x_l = -1, l \neq i} (1 + w_{jl}x_l) \right) x_i = 0$$

Therefore,

$$\Delta w_{ji}(t+1) = \eta d_j \left( \frac{\partial \phi_j}{\partial w_{ji}} \right) = 0$$

In the case of a single mismatched weight,

$$\frac{\partial \phi_j}{\partial w_{ji}} = x_i$$

which is not zero, so the weight adjustment  $\Delta w_{ji}(t+1)$  may or may not be zero, depending on the error  $d_j$ .  $\square$

Since model training starts with small weight values, the initial pattern associated with each channel cannot be exact. When training ends, the channel's pattern may still be inexact because of possible noise, inconsistency, and uncertainty in the data. However, from the proof of the above theorem, we see that when the nonzero weights in the channel's pattern grow larger, the error derivative ( $d_j \frac{\partial \phi_j}{\partial w_{ji}}$ ) generally gets smaller, so does the weight adjustment, and as a result, the pattern becomes more stable and gradually converges to a target pattern. A converged pattern does not move unless there is a near-miss instance (with a single feature mismatch against the pattern) that causes some error in the model output, in which case, the pattern is refined to be a little more general or specific. This analysis explains how the CFRule model ensures the stability of a channel once it is settled in a target pattern. Note that the output weight of a channel with a stable pattern can still be modified toward global error minimization and uncertainty management. In asynchronous parallel convergence, each channel is settled in its own target pattern with a different time frame. Without the above pattern stabilizing property, global convergence is difficult to achieve in the asynchronous mode. This line of

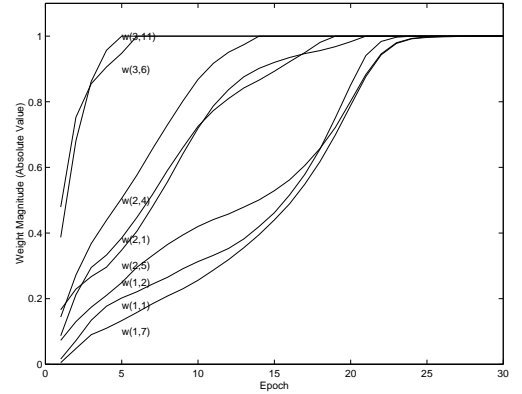


Figure 1: The temporal curves of asynchronous parallel convergence for rule learning.

arguments imply that CFRule admits asynchronous parallel convergence. Theorem 4.1 is unique for CFRule. That property has not been provable for other types of neural networks or learning methods (e.g., [16]).

Asynchronous parallel convergence for rule learning can be illustrated by the example in Section 4.2. Table 2 shows how each channel converges to a target rule in the training course when the model was trained on just 100 random instances (out of  $2^{20}$  possible instances). For instance, given  $\neg x_2$  in the premise of rule 1 (Table 1), we observe the corresponding weight  $w_{1,2}$  of channel 1 converged to  $-1$  (Table 2); also, for  $x_6$  mentioned in rule 3, we see the weight  $w_{3,6}$  of channel 3 converged to 1. Only the significant weights that converge to a magnitude of 1 are shown. Unimportant weights ending up with about zero values are omitted. The convergence behavior can be better visualized in Figure 1. It clearly shows that convergence occurs asynchronously for each channel. It does not matter which channel converges to which rule. This correspondence is determined by the initial weight setting and the data characteristics. Note that given  $k$  channels in the model, there are  $k!$  equivalent permutations in terms of their relative positions in the model. It matters, though, whether the model as a whole converges to all the needed target rules.

## 5 Rule Extraction

As illustrated by the example in Section 4.3, when a channel converges to a target rule, the weights associated with the input attributes contained in the rule's premise grow into large values, whereas the rest of input weights decay to small values. The asymptotic absolute weight values upon convergence approach either 1 or 0 ideally, but this case does not necessarily happen in practical circumstances involving data noise, inconsistency, uncertainty, and inadequate sample sizes. However, in whatever circumstances, it turns out that a simple thresholding mechanism suffices to distinguish important from unimportant weights in the CFRule model. Since the weight absolute values range from 0 to 1, it is reasonable to use 0.5 as the threshold, but this value does not always guarantee

Table 2: Asynchronous parallel convergence to the target rules in the CFRule model. Channels 1, 2, 3 converge to target rules 1, 2, 3, respectively.  $w_{j,i}$  denotes the input weight associated with the input  $x_i$  in channel  $j$ . An epoch consists of a presentation of all training instances.

<i>epoch</i>	$w_{1,1}$	$w_{1,2}$	$w_{1,7}$	$w_{2,1}$	$w_{2,4}$	$w_{2,5}$	$w_{3,6}$	$w_{3,11}$
1	.016	-.073	.005	.144	-.166	.087	.387	.479
5	.202	-.249	.133	.506	-.348	.385	1.00	.948
10	.313	-.420	.256	.868	-.719	.725	1.00	1.00
15	.462	-.529	.440	1.00	-.920	.893	1.00	1.00
20	.851	-.802	.789	1.00	-.983	1.00	1.00	1.00
25	1.00	-.998	.996	1.00	-1.00	1.00	1.00	1.00
30	1.00	-1.00	1.00	1.00	-1.00	1.00	1.00	1.00

optimal performance. How to search for a good threshold in a continuous range is difficult. Fortunately, thanks to the quantizability nature of the system adopting the CF model [9], only a handful of values need to be considered. Our research has narrowed it down to four candidate values: 0.35, 0.5, 0.65, and 0.8. A larger threshold makes extracted rules more general, whereas a smaller threshold more specific. In order to lessen data overfitting, our heuristic is to choose a higher value as long as the training error is acceptable. Using an independent cross-validation data set is a good idea if enough data is available. The rule extraction algorithm is formulated below.

*The CFRule Rule Extraction Algorithm*

- Select a rule extraction threshold  $r$  ( $0 < r < 1$ ).
- For each channel  $j$ ,
  1.  $P := nil$  (an empty set)
  2.  $C :=$ the target class
  3. Normalize the input weights  $w_{ji}$ 's so that the maximum weight absolute value is 1.
  4. For each input weight  $w_{ji}$  ( $1 \leq i \leq d$ ,  $d$ : the input dimensionality),
    - a. If  $w_{ji} \geq r$ , then add  $x_i$  to  $P$ .
    - b. If  $w_{ji} \leq -r$ , then add  $\neg x_i$  to  $P$ .
    - c. Else, do nothing.
  5. Form a rule: "IF  $P$ , THEN  $C$  with CF =  $u_j$ " ( $u_j$ : the output weight based on the rule).
- Remove subsumed rules and rules with low CFs.

The threshold-based algorithm described here is fundamentally different from the search-based algorithm in neural network rule extraction [7, 9, 20]. The main advantage with the threshold-based approach is its linear computational complexity with the total number of weights, in contrast to polynomial or even exponential complexity incurred by the search-based approach. Furthermore, the former approach obviates the need of a special training, pruning, or approximation procedure commonly used in

the latter approach for complexity reduction. As a result, the threshold-based, direct approach should produce better and more reliable rules. Notice that this approach is not applicable to the ordinary sigmoid-function neural network where knowledge is entangled. The admissibility of the threshold-based algorithm for rule extraction in CFRule can be ascribed to the CF-combining function.

## 6 Applications

Two benchmark data sets were selected to demonstrate the value of CFRule on practical domains. The promoter data set is characterized by high dimensionality relative to the sample size, while the hepatitis data has a lot of missing values. Thus, both pose a challenging problem.

The decision-tree-based rule generator system C4.5 [18] was taken as a control since it (and with its later version) is the currently most representative (or most often used) rule learning system, and also the performance of C4.5 is optimized in a statistical sense.

### 6.1 Promoter Recognition in DNA

In the promoter data set [23], there are 106 instances with each consisting of a DNA nucleotide string of four base types: A (adenine), G (guanine), C (cytosine), and T (thymine). Each instance string is comprised of 57 sequential nucleotides, including fifty nucleotides before (minus) and six following (plus) the transcription site. An instance is a positive instance if the promoter region is present in the sequence, else it is a negative instance. There are 53 positive instances and 53 negative instances, respectively. Each position of an instance sequence is encoded by four bits with each bit designating a base type. So an instance is encoded by a vector of 228 bits along with a label indicating a positive or negative instance.

In the literature of molecular biology, promoter (of prokaryotes) sequences have average constitutions of -TTGAC- and -TATAAT-, respectively, located at so-called minus-35 and minus-10 regions [14], as shown in Table 3.

Table 3: The promoter (of prokaryotes) consensus sequences.

<i>Region</i>	<i>DNA Sequence Pattern</i>
Minus-35	@-36=T @-35=T @-34=G @-33=A @-32=C @-31=A
Minus-10	@-13=T @-12=A @-11=T @-10=A @-9=A @-8=T

The CFRule model in this study had 3 channels, which were the minimal number of channels to bring the training error under 0.02 upon convergence. Still, the model is relatively underdetermined because of the low ratio of the number of instances available for training to the input dimension. However, unlike our previous approach [9], we did not use any pruning strategy. The model had to learn to cope with high dimensionality by itself. The learning rate was set to 0.2, and the rule extraction threshold 0.5 (all these are default values). The model was trained on the training data under the MCRO strategy and then tested on the test data. The stopping criterion for training was the drop of MSE (mean squared error) less than a small value per epoch. Rules were extracted from the trained model.

Cross-validation is an important means to evaluate the ability of learning. Domain validity is indicated if rules learned based on some data can be well applied to other data in the same domain. In the two-fold cross-validation experiment, the 106 instances were randomly divided equally into two subsets. CFRule and C4.5 used the same data partition. The rules learned on one subset were tested by the other and vice versa. The average prediction error rate on the test set was defined as the cross-validation *rule* error rate. The cross-validation experiment with CFRule was run 5 times, each with a different initial weight setting. The average cross-validation error was reported. CFRule had a significantly smaller cross-validation rule error rate than C4.5 (12.8% versus 23.9%, respectively), as shown in Table 4. Note that the prediction accuracy and the error rate were measured based on exact symbolic match. That is, an instance is predicted to be in the concept only if it matches exactly any rule of the concept, else it is not in the concept. If, however, prior domain knowledge is used and exact symbolic match is not required, the error rate based on leave-one-out can be as low as 2% [7].

The data for this research are available from a machine learning database located in the University of California at Irvine with an ftp address at ftp.ics.uci.edu/pub/machine-learning-databases.

## 6.2 Hepatitis Prognosis Prediction

In the data set concerning hepatitis prognosis<sup>1</sup>, there are 155 instances, each described by 19 attributes. Contin-

<sup>1</sup>This data set is an old version previously used in our research work [7].

Table 4: The average two-fold cross-validation error rates of the rules learned by C4.5 and CFRule, respectively.

<i>Domain</i>	<i>C4.5</i>	<i>CFRule</i>
Promoters (without prior knowledge)	23.9%	12.8%
Hepatitis	7.1%	5.3%

uous attributes were discretized, then the data set was randomly partitioned into two halves (78 and 77 cases), and then cross-validation was carried out. CFRule and C4.5 used exactly the same data to ensure fair comparison. The CFRule model for this problem consisted of 2 channels. Again, CFRule was superior to C4.5 based on the cross-validation performance (see Table 4).

## 7 Conclusions

If global optimization is a main issue for automated rule discovery from data, then current machine learning theories do not seem adequate. For instance, the decision-tree and neural-network based algorithms, which dodge the complexity of exhaustive search, guarantee only local but not global optimization. In this paper, we introduce a new machine learning theory based on multi-channel parallel adaptation that shows great promise in learning the target rules from data by parallel global convergence. The basic idea is that when a model consisting of multiple parallel channels is optimized according to a certain global error criterion, each of its channels converges to a target rule. While the theory sounds attractive, the main question is how to implement it. In this paper, we show how to realize this theory in a learning system named CFRule.

CFRule is a parallel weight-based model, which can be optimized by weight adaptation. The parameter adaptation rule follows the gradient-descent idea which is generalized in a multi-level parallel context. However, the central idea of the multi-channel rule-learning theory is not about how the parameters are adapted but rather, how each channel can converge to a target rule. We have noticed that CFRule exhibits the necessary conditions to ensure such convergence behavior. We have further found that the CFRule’s behavior can be attributed to the use of the CF (certainty factor) model for combining the inputs and the channels.

Since the gradient descent technique seeks only a local minimum, the learning model may well be settled in a solution where each rule is optimal in a local sense. A strategy called multi-channel regression-based optimization (MCRO) has been developed to address this issue. This strategy has proven effective by statistical validation.

We have formally proven two important properties that account for the parallel rule-learning behavior of CFRule. First, we show that any given rule set can be explicitly and precisely encoded by the CFRule model. Secondly, we show that once a channel is settled in a target rule, it barely moves. These two conditions encourage the model



to move toward the target rules. An empirical weight convergence graph clearly showed how each channel converged to a target rule in an asynchronous manner. Notice, however, we have not been able to prove or demonstrate this rule-oriented convergence behavior in other neural networks.

We have then examined the application of this methodology to DNA promoter recognition and hepatitis prognosis prediction. In both domains, CFRule is superior to C4.5 (a rule-learning method based on the decision tree) based on cross-validation. Rules learned are also consistent with knowledge in the literature.

In conclusion, the multi-channel parallel adaptive rule-learning theory is not just theoretically sound and supported by computer simulation but also practically useful. In light of its significance, this theory would hopefully point out a new direction for machine learning and data mining.

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