Some Nonparametric Hybrid Predictive Models: Asymptotic Properties and Applications

by

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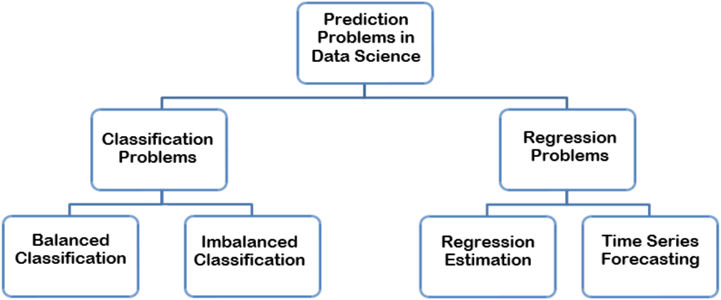
Outline of the talk

- Motivation
- Chapters
- Publications
- Acknowledgements
- References

Motivation

"**Prediction** is very difficult, especially if it's about the future" - Niels Bohr, Father of Quantum Mechanics.



Prediction Problems in Data Science

Classification Problems

Regression Problems

Balanced Classification

Imbalanced Classification

Regression Estimation

Time Series Forecasting

Motivation

- Predictive modelling approaches are used in the fields of statistics and machine learning, mainly for their accuracy and ability to deal with complex data structures.
- In this thesis, we have developed some novel Hybrid Predictive models motivated by the applied problems from the domain of Business Analytics, Quality Control, Macroeconomics, and Software Reliability. More precisely, we have considered the following prediction problems:

1. Feature Selection cum Classification Problem.
2. Imbalanced Classification Problem.
3. Nonparametric Regression estimation problem.
4. Designing Regression Model Combining Frequentist and Bayesian Methods.
5. Designing Forecasting Model for Nonstationary and Nonlinear Time Series data.

Motivation

- Primary motivation of this thesis comes from the real-world data sets, with a variety of data types, such as business, macroeconomics, process efficiency improvement, water quality control, and software defect prediction.
- As a secondary motivation, we emphasis on the development of hybrid models that are scalable (the size of the data does not pose a problem), robust (work well in a wide variety of problems), accurate (achieve higher predictive accuracy), statistically sound (have desired asymptotic properties), and easily interpretable.
- The newly developed hybrid methods are shown to outperform the current state-of-the-arts and overcome the deficiencies of the hybrid models available in the literature.
- Both theoretical (asymptotic results) and computational aspects of the proposed hybrid frameworks are studied.

Thesis Overview

- Chapter 1: Introduction
- Chapter 2: Preliminaries
- Chapter 3: A Nonparametric Hybrid Model for Pattern Classification
- Chapter 4: Hellinger Net : A Hybrid Model for Imbalanced Learning
- Chapter 5: A Distribution-free Hybrid Method for Regression Modeling
- Chapter 6: Bayesian Neural Tree Models for Nonparametric Regression
- Chapter 7: A Hybrid Time Series Model for Macroeconomic Forecasting
- Chapter 8: Conclusions and Future Works

CHAPTER 1: INTRODUCTION

Popular Prediction Models

- Linear Regression (Galton, 1875).
- Linear Discriminant Analysis (R.A. Fisher, 1936).
- Logistic Regression (Berkson, JASA, 1944).
- k-Nearest Neighbor (Fix & Hodges, 1951).
- Parzens Density Estimation (E Parzen, AMS, 1962)
- ARIMA Model (Box and Jenkins, 1970).
- Classification and Regression Tree (Breiman et al., 1984).
- Artificial Neural Network (Rumelhart et al., 1985).
- MARS (Friedman, 1991, Annals of Statistics).
- SVM (Cortes & Vapnik, Machine learning, 1995)
- Random forest (Breiman, 2001).
- Deep Convolutional Neural Nets (Krizhevsky, Sutskever, Hinton, NIPS 2012).
- GAN (Goodfellow et al., NIPS 2014).
- Deep Learning (LeCun, Bengio, Hinton, Nature 2015).
- Bayesian Deep Neural Network (Y. Gal, Islam, Zoubin, ICML 2017).

Need for Hybridization

- Statistical issue: It is often the case that the model space is too large to explore for limited training data, and that there may be several different models giving the same accuracy on the training data. The risk of choosing the wrong model can be reduced by combining two models, like CART and ANN.

- Representation issue: In many learning tasks, the true unknown hypothesis could not be represented by any hypothesis in the hypothesis space. By hybridization, it may be possible to expand the space of representable functions. Thus the learning algorithm may be able to form a more accurate approximation to the true unknown hypothesis.

- Computational issue: Many learning algorithms perform some kind of local search that may get stuck in local optima. Even if there are enough training data, it may still be challenging to find the best hypothesis. By combining two or more models, the risk of choosing a wrong local minimum can be reduced.

Ensemble & Hybrid Models

- Problem: Single models have the drawbacks of sticking to local minimum or over-fitting the data set, etc.
- Ensemble models are such where predictions of multiple models are combined together to build the final model.
- Examples: Bagging, Boosting, Stacking and Voting Method
- Caution: But ensembles dont always improve accuracy of the model but tends to increase the error of each individual base classifier.
- Hybrid models are such where more than one models are combined together.
- It overcomes the limitations of single models and reduce individual variance & bias, thus improve the performance of the model.
- Caution: To build a good ensemble classifier the base classifier needs to be simple, as accurate as possible, and distinct from the other classifier used.
- Desired: Interpretability, Less Complexity, Less Tuning Parameters, high accuracy.

Popular Hybrid Prediction Models

- Perceptron Trees (Utgoff, AAAI, 1988).
- Entropy Nets (Sethi, Proceeding of IEEE,1990).
- Neural trees (Sirat & Nadal, Network, 1990).
- Sparse Perceptron Trees (Jackson, Craven, NIPS, 1996).
- SVM Tree Model (Bennett et al., NIPS, 1998)
- Hybrid DT-ANN Model (Jerez-Aragones et al., 2003, AI in Medicine)
- Flexible Neural Tree (Chen et al., Neurocomputing, 2006)
- Hybrid DT-SVM Model (Sugumaran et al,, Mechanical Systems and Signal Processing, 2007).
- Hybrid CNNSVM Classifier (Niu et al., PR, 2012).
- Convolutional Neural Support Vector Machines (Nagi et al., IEEE ICMLA, 2012).
- Hybrid DT model utilizing local SVM (Dejan et al., IJPR, 2013).
- Neural Decision Forests (Bulo, Kontschieder, CVPR, 2014).
- Deep Neural Decision Forests (Kontschieder, ICCV, 2015).
- Soft Decision Tree (Frosst, Hinton, Google AI, 2017).
- Deep Neural Decision Trees (Yang et al., ICML, 2018).

Some Drawbacks of the Existing Hybrid Models

- Theoretical Robustness: Regardless of the practical use of SDT and neural trees, theoretical properties like universal consistencies of these hybrid methods are unknown. Thus, one needs to analyze the data complexity for splitting, which leads to more accurate classification in the neural trees node.

- High-dimensional set-up: Accurate classification of high dimensional feature space leads to more depth trees, thus achieving less depth neural trees require more complex computations at each node.

- Small Sample Size and Interpretability: The previously used hybrid models sometimes over-fit for small or moderate sample-sized data sets. In DNDT, each node in their oblique decision tree involves all features rather than a single feature, which renders the model uninterpretable.

Chapter 2: Preliminaries

Decision Trees

- Decision tree is defined by a hierarchy of rules (in form of a tree).
- Rules from the internal nodes of the tree are called root nodes
- Each rule (internal node) tests the value of some feature.
- Labeled training data is used to construct the Decision tree. The tree need not to be always a binary tree.
- CART (Breiman et al., 1984), RF (Breiman, 2001), BART (Chipman et al., 2010).
- CART is a greedy divide-and-conquer algorithm.
- Attributes are selected on the basis of an impurity function (e.g., IG for Classification & MSE for Regression).
- **Pros:** Built-in feature selection mechanism, Comprehensible, easy to design, easy to implement, good for structural learning.
- **Cons:** Too many rules loose interpretability, risk of over-fitting, sticking to local minima.

Introduction: Graphical Interpretation

- Let $\underline{X}$ be the space of all possible values of p features and C be the set of all possible binary outcomes. We are given a training sample with n observations $L = \{(X_1, C_1), (X_2, C_2), \dots, (X_n, C_n)\}$, where $X_i = (X_{i1}, X_{i2}, \dots, X_{ip}) \in \underline{X}$ and $C_i \in C$.
- Also let $\Omega = \{\omega_1, \omega_2, \dots, \omega_k\}$ be a partition of the feature space $\underline{X}$. We denote $\widetilde{\Omega}$ as one such partition of Ω. Define $L_{\omega_i} = \{(X_i, C_i) \in L : X_i \in \omega_i, C_i \in C\}$ as the subset of L induced by ω_i and let $L_{\widetilde{\Omega}}$ denote the partition of L induced by $\widetilde{\Omega}$.
- Now, let us define $\widehat{L}$ to be the space of all learning samples and $\mathbb{D}$ be the space of all partitioning classification function, then $\Phi : \widehat{L} \to \mathbb{D}$ such that $\Phi(L) = (\psi \circ \phi)(L)$, where ϕ maps L to some induced partition $(L)_{\widetilde{\Omega}}$ and ψ is an assigning rule which maps $(L)_{\widetilde{\Omega}}$ to d on the partition $\widetilde{\Omega}$.
- The most basic reasonable assigning rule ψ is the plurality rule $\psi_{pl}(L_{\widetilde{\Omega}}) = d$ such that if $x \in \omega_i$, then $d(\underline{x}) = \arg\max_{c \in C} |L_{c,\omega_i}|$.
- For any random variable X and set A, let $\eta_{n,X}(A) = \frac{1}{n}\sum_{i=1}^{n} I(X_i \in A)$ be the empirical probability that $X \in A$ based on n observations and I denotes the indicator function.

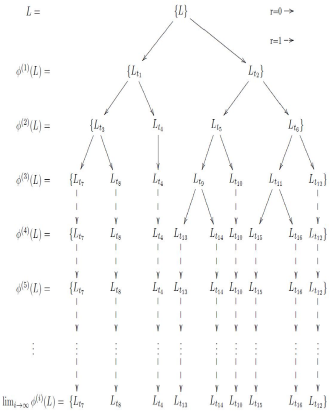


Fig: Graphical interpretation of tree structured model.

Artificial Neural Networks

- ANN is composed of several perceptron-like units arranged in multiple layers.
- Consists of an input layer, one or more hidden layer, and an output layer.
- Nodes in the hidden layers compute a nonlinear transform of the inputs.
- **Universal Approximation Theorem (Hornik, 1989)**: A one hidden layer FFNN with sufficiently large number of hidden nodes can approximate any function.
- **Pros:** Able to learn any complex nonlinear mapping or approximate any continuous function.
- **Pros:** No prior assumption about the data distribution or input-output mapping function.
- **Cons:** When applied to limited data can overfit the training data and lose generalization capability
- **Cons:** Training ANN is time-consuming and selection of the network topology lack theoretical background, often "trial and error" matter.

Statistical Learning Theory: Consistency

- Statistical learning theory (SLT) studies mathematical foundations for machine learning models, originated in late 1960s.
- Basic concept of Consistency: A learning rule, when presented more and more training examples → the optimal solution.

Definition (Consistency)

Given an infinite sequence of training points $(X_i, Y_i)_{i \in N}$ with μ. For each $n \in N$, let f_n be a classifier for the first n training points. The learning algorithm is called consistent with respect to μ if the risk $R(f_n)$ converges to the risk $R(f_{Bayes})$, that is for all $\epsilon > 0$,

$$\mu(R(f_n) - R(f_{Bayes}) > \epsilon) \to 0 \textit{ as } n \to \infty.$$

Definition (Universally Consistency)

The learning algorithm is called universally consistent if it is consistent for all probability distributions μ.

Statistical Learning Theory in Decision Trees & Neural Networks

- Consistency of data driven histogram methods (Lugosi & Nobel, 1996, Annals of Statistics).
- A Fast, Bottom-Up Decision Tree Pruning Algorithm with Near-Optimal Generalization (Kearns, Mansour, ICML, 1998)
- Generalization Bounds for Decision Trees (Mansour et al., 2000, COLT).
- Consistency of Online Random Forest (Denil et al., 2013, ICML).
- Consistency of Random Forest (Scornet et al., 2015, Ann. Stat.).
- Strong Universal Consistency of FFNN Classifier (Lugosi & Zeger 1995, IEEE Information Theory).
- Approximation properties of ANN (Mhaskar, 1993, Advances in Computational Mathematics).
- Prediction Intervals for Artificial Neural Networks (Hwang, Ding, 1997, JASA)
- Provable approximation properties for DNN (Shaham et al., 2018, Applied & Computational Harmonic Analysis).
- On Deep Learning as a remedy for the curse of dimensionality (Bauer, Kohler, 2019, Ann. Stat.).

Consistency of data-driven histogram methods for density estimation and classification

Theorem (Lugosi and Nobel, 1996, Annals of Statistics)

Let $(\underline{X}, \underline{Y})$ be a random vector taking values in $\mathbb{R}^p \times C$ and L be the set of first n outcomes of $(\underline{X}, \underline{Y})$. Suppose that Φ is a partition and classification scheme such that $\Phi(L) = (\psi_{pl} \circ \phi)(L)$, where ψ_{pl} is the plurality rule and $\phi(L) = (L)_{\tilde{\Omega}_n}$ for some $\tilde{\Omega}_n \in \mathcal{T}_n$, where $\mathcal{T}_n = \{\phi(\ell_n) : P(L = \ell_n) > 0\}$. Also suppose that all the binary split functions in the question set associated with Φ are hyperplane splits. As $n \to \infty$, if the following regularity conditions hold:

$$\frac{\lambda(\mathcal{T}_n)}{n} \to 0 \tag{0.1}$$

$$\frac{log(\triangle_n(\mathcal{T}_n))}{n} \to 0 \tag{0.2}$$

and for every $\gamma > 0$ and $\delta \in (0, 1)$,

$$\inf_{S \subseteq \mathbb{R}^p : \eta_x(S) \geq 1-\delta} \eta_x(x : diam(\tilde{\Omega}_n[x] \cap S) > \gamma) \to 0 \tag{0.3}$$

with probability 1. then Φ is risk consistent.

Eqn. (0.2) is the sub-linear growth of the number of cells, Eqn. (0.3) is the sub-exponential growth of a combinatorial complexity measure, and Eqn. (0.4) is the shrinking cell condition.

Consistency Results for Neural Network Classifier

Theorem (Lugosi & Zeger, 1995, IEEE Information Theory)

Consider a neural network with one hidden layer with bounded output weight having k hidden neurons and let σ be a logistic squasher. Let $F_{n,k}$ be the class of neural networks defined as

$$F_{n,k} = \left\{ \sum_{i=1}^{k} c_i \sigma(a_i^T z + b_i) + c_0 : k \in \mathbb{N}, a_i \in \mathbb{R}^{dm}, b_i, c_i \in \mathbb{R}, \sum_{i=0}^{k} |c_i| \leq \beta_n \right\}$$

and let ψ_n be the function that minimizes the empirical L_1 error over $\psi_n \in F_{n,k}$. It can be shown that if k and β_n satisfy

$$k \rightarrow \infty, \quad \beta_n \rightarrow \infty, \quad \frac{k\beta_n^2 log(k\beta_n)}{n} \rightarrow 0$$

then the classification rule

$$g_n(z) = \begin{cases} 0, & \text{if } \psi_n(z) \leq 1/2. \\ 1, & \text{otherwise.} \end{cases} \tag{0.4}$$

is universally consistent.

For universal convergence, the class over which the minimization is performed has to be defined carefully. Above theorem shows that this may be achieved by neural networks with k nodes, in which the range of output weights $c_0, c_1, \ldots, c_k$ is restricted.

Introduction: Perceptron Trees (AAAI, 1988)

- Perceptron trees are composed of three basic steps:

  (a) Converting a DT into rules.
  (b) Constructing a two hidden layered NN from the rules.
  (c) Training the MLP using gradient descent backpropagation (Rumelhart, Hinton (1988).

- In decision trees, the overfitting occurs when the size of the tree is too large compared to the number of training data.

- Instead of using pruning methods (removing child nodes), PT employs a backpropagation NN to give weights to nodes according to their significance.

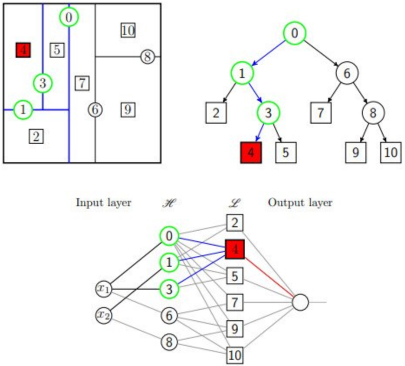


Fig: Graphical Representation of Perceptron Trees Model [Paul Utgoff, 1988, AAAI]

Introduction: SVM Tree Model (NIPS, 1998)

- SVM are generalized to decision trees. SVM is used for each decision in the tree.
- The "optimal" decision tree is characterized, and both a primal and dual space formulation for constructing the tree are introduced.
- The model results in a simple decision trees with multivariate linear or nonlinear decisions.
- Consistency results are yet to be proved and can be extended for different problems (Interesting Problem!).

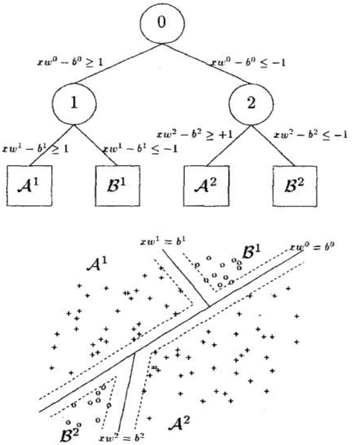
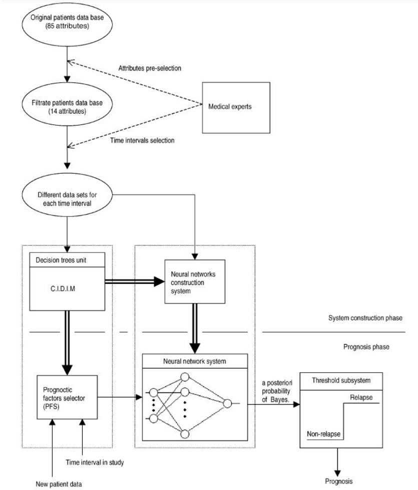


Fig: SVM Formulation for Decision Trees: A logical and geometric depiction of a decision tree with optimal margins [Bennett ET AL., 1998, NIPS]

Introduction: Hybrid DT-ANN Model (AI in Medicine, 2003)

- The DT unit leads to the selection of the most significant prognostic factors from the patients' database for every time interval.
- The NN system computes an attributes set from the prognostic factors selector giving a value corresponding to the a posteriori probability of relapse for the patient under study.
- Useful when (a) data present an important number of attributes with missing values, (b) the prognostic factors' significance is not the same over the time of patient follow-up, and the utilisation of survival estimate techniques is not very advisable.
- Promising area for Biostatisticians.



Original patients data base (85 attributes)

Attributes pre-selection

Medical experts

Filtrate patients data base (14 attributes)

Time intervals selection

Different data sets for each time interval

Decision trees unit

C.I.D.I.M

Neural networks construction system

System construction phase

Prognosis phase

Neural network system

Prognoctic factors selector (PFS)

a posteriori probability of Bayes.

Threshold subsystem

Relapse

Non-relapse

Time interval in study

New patient data

Prognosis

Fig: A combined ANN and DT model for prognosis of breast cancer [Jerez-Aragones et al., 2003, AI in Medicine]

Introduction: Hybrid DT-SVM Model (MSSP, 2007)

- DT is used to identify the best features from a given set of samples for the purpose of classification.
- Proximal Support Vector Machine (PSVM) which has the capability to efficiently classify the faults are used for classification task using the DT identified features.
- In general, the approach can be used for feature selection in any domain.
- Simple, interpretable, but lacks accuracy in some typical problems.

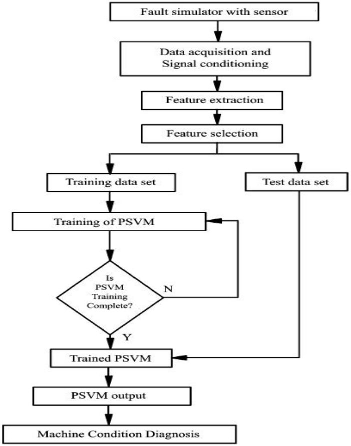

Fault simulator with sensor
Data acquisition and Signal conditioning
Feature extraction
Feature selection
Training data set
Test data set
Training of PSVM
Is PSVM Training Complete?
N
Y
Trained PSVM
PSVM output
Machine Condition Diagnosis

Fig: Feature selection using Decision Tree and classification through Proximal Support Vector Machine for fault diagnostics of roller bearing [Sugumaran et al., 2007, Mechanical Systems & Signal Processing]

Introduction: DNDF for Image Data Sets (ICCV, 2015)

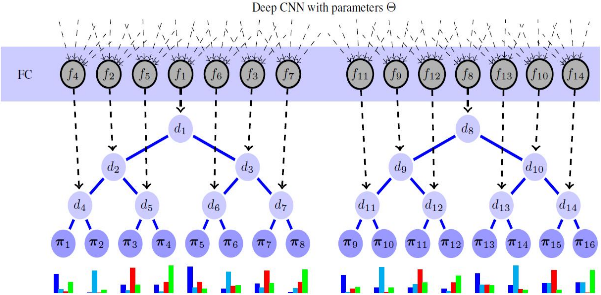

Deep CNN with parameters Θ
FC
f_4 f_2 f_5 f_1 f_6 f_3 f_7 f_{11} f_9 f_{12} f_8 f_{13} f_{10} f_{14}
d_1 d_8
d_2 d_3 d_9 d_{10}
d_4 d_5 d_6 d_7 d_{11} d_{12} d_{13} d_{14}
π_1 π_2 π_3 π_4 π_5 π_6 π_7 π_8 π_9 π_{10} π_{11} π_{12} π_{13} π_{14} π_{15} π_{16}

Fig: Deep neural decision forests [Kontschieder et al., 2015, ICCV]

Description: Deep CNN with variable number of layers, subsumed via parameters θ.
FC block: Fully Connected layer used to provide functions $f_n(;\theta)$. Each output of f_n is brought in correspondence with a split node in a tree, eventually producing the routing (split) decisions $d_n(x) = \sigma(f_n(x))$. The order of the assignments of output units to decision nodes can be arbitrary (the one we show allows a simple visualization).
The circles at bottom correspond to leaf nodes, holding probability distributions π.

Chapter 3: A Nonparametric Hybrid Model for Pattern Classification

Publications:

1. Tanujit Chakraborty, Ashis Kumar Chakraborty, and C. A. Murthy. "A nonparametric ensemble binary classifier and its statistical properties", **Statistics & Probability Letters**, 149 (2019): 16-23. **(Read Online)**

2. Tanujit Chakraborty, Swarup Chattopadhyay, and Ashis Kumar Chakraborty. "A novel hybridization of classification trees and artificial neural networks for selection of students in a business school", **Opsearch**, 55 (2018): 434-446. **(Read Online)**

Motivating Problem

- Placement of MBA student is a serious concern for Private B-Schools.

- The data is collected from a private business school which receives applications from across the country for the MBA program and admits a pre-specified number of students every year.

- Authorities want us to come up with a model that can help them to predict whether a student will be placed or not on certain characteristics of that students provided at the time of admission.

- Selecting a wrong student may increase the number of unplaced students. Also, more the number of unplaced students more is the negative impact on the institutes reputation.

Business School Data

- The data set comprises of several parameters of passed out students profile (collected at the time of admission) along with their placement information (collected at the end of the MBA program).
- The data set comprise of several parameters of passed out students' profile along with their placement information (on average 60% students got placed in last 5 years).
- The data contains 24 explanatory variables out of which 7 are categorical variables. The response variable (Placement) indicate whether the student got placed or not.

Table: Sample business school data set.

ID	Gender	SSC Percentage	HSC Percentage	DEGREE Percentage	E.Test Percentile	SSC Board	HSC Board	HSC Stream	Placement
1	M	68.4	85.6	72	70	ICSE	ISC	Commerce	Y
2	M	59	62	50	79	CBSE	CBSE	Commerce	Y
3	M	65.9	86	72	66	Others	Others	Commerce	Y
4	F	56	78	62.4	50.8	ICSE	ISC	Commerce	Y
5	F	64	68	61	24.3	Others	Others	Commerce	N
6	F	70	55	62	89	Others	Others	Science	Y
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.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.

Scope of the Problem

- **Goal**: We would like to come up with a model that can help the authorities of a business school to predict whether a student will be placed or not based on certain characteristics of that student at the time of admission to the professional course.
- **Scope**: Feature Selection (selection of important students' characteristics) cum data classification (a system that will give judgements based on the characteristics of new applicants to their MBA program).
- **Previous works**: Dean's dilemma problem is very popular in Educational data mining. There are various literature available in the field where data mining techniques like logistic regression, LDA, DT, ANN, kNN, SVM, RF, etc have been employed to model students' admission, students' placements.
- Pena-Ayala A (2014) **Educational data mining: A survey and a data mining-based analysis of recent works**. Expert systems with applications, Elsevier, 41(4):14321462 provides a survey of all the techniques used in similar problems.

Development of an Ensemble Model

- First, apply classification tree algorithm to train and build a decision tree model that extracts important features.
- Feature selection model is generated by decision tree and it also shortlists the important features and filters out the rest.
- The prediction result of CT algorithm is used as an additional feature in the input layer of ANN model.
- Export important input variables along with additional input variable to the appropriate ANN model and network is generated.
- Run ANN algorithm till satisfactory accuracy is reached by optimizing weights and number of hidden layer neurons. Then the classifier will be ready to use.

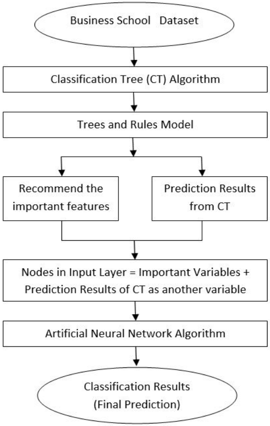

Business School Dataset
Classification Tree (CT) Algorithm
Trees and Rules Model
Recommend the important features
Prediction Results from CT
Nodes in Input Layer = Important Variables + Prediction Results of CT as another variable
Artificial Neural Network Algorithm
Classification Results (Final Prediction)

Fig: Flowchart of the Ensemble Model

But...

- What will be the optimal Choice of the number of hidden nodes for the model? (Trial and Error!)
- Theoretical Consistency of the Model? (Statistical Learning Theory!)
- Importance of CT output in the second stage of the ensemble model? (Experimental or Theoretical Justification!)
- Experimental Evaluation and comparative study with single and hybrid ensemble models? (Important!)
- Can this model be useful for practitioner working in other disciplines but on similar types of problems? (Very Important!)

Improved Version of the Proposed Model

- First, apply the CT algorithm to train and build a decision tree and record important features.
- Using important input variables obtained from CT along with an additional input variable (CT output), a FFNN model (with one hidden layer) is generated.
- The optimum number of neurons in the hidden layer of the model to be chosen as $O\left(\sqrt{n/d_m log(n)}\right)$ [to be discussed], where n, d_m are number of training samples and number of input features in ANN model, respectively.

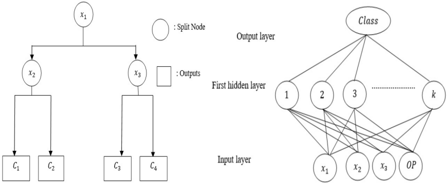


Figure: Graphical Presentation of the proposed ensemble model

Merits

- Can select important features from the data set;
- Suitable for Feature Selection cum Classification Problems with limited data sets;
- Useful for high dimensional feature spaces in the data sets;
- Simple and Easily interpretable;
- “white-box-like” model, fast in implementation.

On Theoretical Consistency

- A consistent rule guarantees us that taking more samples essentially suffices to roughly reconstruct the unknown distribution of (X, Y).

- A binary tree-based classification and partitioning scheme Φ is defined as an assignment rule applied to the limit of a sequence of induced partitions $\phi^{(i)}(L)$, where $\phi^{(i)}(L)$ is the partition of the training sample L induced by the partition $(\phi_i \circ \phi_{i-1} \circ .... \circ \phi_1)(\underline{X})$.

- We need to show that CT scheme are well defined, which will be possible only if there exists some induced partition $L^{'}$ such that $\lim_{i \to \infty} \phi^{(i)}(L) = L^{'}$.

- If each cell of L_{ω_i} has cardinality $\geq k_n$ and $\frac{k_n}{log(n))} \to \infty$, then CT is said to be risk consistent.

- Theorem (below) along with the consistency results of FFNN model ensures the universal consistency of the proposed hybrid model.

On Theoretical Consistency

Lemma (Chakraborty et al., 2019, Statistics & Probability Letters)

If L is a training sample and $\phi^{(i)}$ is defined as above, then there exists $N \in \mathbb{N}$ such that for $n \geq N$

$$\phi^{(n)}(L) = \lim_{i \to \infty} \phi^{(i)}(L)$$

Theorem (Chakraborty et al., 2019, Statistics & Probability Letters)

Suppose $(\underline{X}, \underline{Y})$ be a random vector in $\mathbb{R}^p \times \; C$ and L be the training set consisting of n outcomes of $(\underline{X}, \underline{Y})$. Let Φ be a classification tree scheme such that $\Phi(L) = (\psi_{pl} \circ \lim_{i \to \infty} \phi^{(i)})(L)$ where, ψ_{pl} is the plurality rule and $\phi(L) = (L)_{\tilde{\Omega}_n}$ for some $\tilde{\Omega}_n \in \mathcal{T}_n$, where

$$\mathcal{T}_n = \{\lim_{i \to \infty} \phi^{(i)}(\ell_n) : P(L = \ell_n) > 0\}.$$

Suppose that all the split function in CT in the question set associated with Φ are axis-parallel splits. Finally if for every n and $w_i \in \tilde{\Omega}_n$, the induced subset L_{w_i} has cardinality $\geq k_n$, where $\frac{k_n}{log(n))} \to \infty$ and shrinking cell condition holds true, then Φ is risk consistent.

On the choice of Number of Hidden Neurons

Lemma (Chakraborty et al., 2019, Statistics & Probability Letters)

Assume that there is a compact set $E \subset \mathbb{R}^{d_m}$ such that $Pr\{Z \in E\} = 1$ and the Fourier transform $\widetilde{P_0}(w)$ of $P_0(z)$ satisfies $\int_{\mathbb{R}^{d_m}} |\omega||\widetilde{P_0}(\omega)|d\omega < \infty$ then $\inf_{\psi \in F_{n,k}} E\Big(f(Z,\psi) - P_0(Z)\Big)^2 \leq \frac{c}{k}$, where c is a constant depending on the distribution.

Proposition (Chakraborty et al., 2019, Statistics & Probability Letters)

For a fixed d_m, let $\psi_n \in F_c$. The neural network satisfying regularity conditions of strong universal consistency and if the conditions of the above lemma holds, then the optimal choice of k is $O\left(\sqrt{\frac{n}{d_m log(n)}}\right)$.

- For practical use, if the data set is limited, the recommendation is to use $k = \left(\sqrt{\frac{n}{d_m log(n)}}\right)$ for achieving utmost accuracy of the propose model.

Importance of CT output in neural net

- CT output also plays an important role in further modeling. It actually improves the performance of the model at a significant rate (can be shown using experimental results).
- We can use one hidden layer in ANN model due to the incorporation of CT output as an input information in ANN.
- CT predicted results provide some direction for the second stage modelling using ANN.
- Tree output estimates are probabilistic estimates, not from a direct mathematical or parametric model, thus direct correlationship with variables can't be estimated.
- It should be noted that one-hidden layer neural networks yield strong universal consistency and there is little theoretical gain in considering two or more hidden layered neural networks (Devroye, IEEE IT, 2013).

Measure of Importance of CT output

To see the importance of CT given classification results as a relevant feature, we introduce a non-linear measure of correlation between any feature and the actual class levels, namely C-correlation (Yu and Liu, 2004, JMLR) as follows:

Definition (C-correlation)

It is the correlation between any feature F_i and the class levels C, denoted by $SU_{F_i,C}$. Symmetrical uncertainty (SU) is defined as follows:

$$SU(X,Y) = 2\left[\frac{H(X) - H(X|Y)}{H(X) + H(Y)}\right] \tag{0.5}$$

where, $H(X)$ is the entropy of a variable X and $H(X|Y)$ is the entropy of X while Y is observed.

- We can decide a feature to be highly correlated with class C if $SU_{F_i,C} > \beta$, where β is a relevant threshold to be determined by user.
- While experimentation, we can check whether CT output can be taken as a non-redundant feature for further model building.

Application on Business School Data

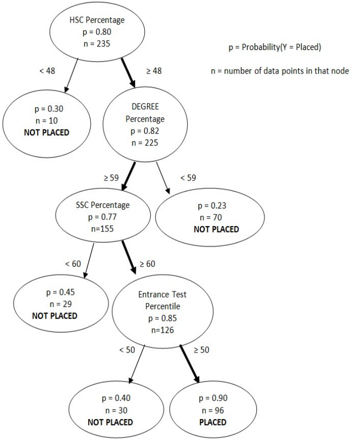


Fig: Decision Tree Diagram

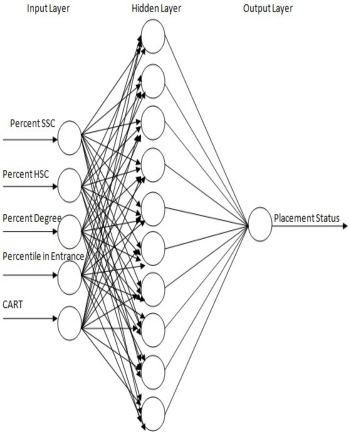


Fig: Ensemble CT-ANN Model Diagram

Performance Evaluation

Popularly used performance metric are:

Precision=$\frac{TP}{TP+FP}$; Recall=$\frac{TP}{TP+FN}$;

F-measure $=2\frac{(Precision.Recall)}{(Precision+Recall)}$; Accuracy $=\frac{(TP+TN)}{(TP+TN+FP+FN)}$;

TP (True Positive): correct positive prediction; FP (False Positive): incorrect positive prediction; TN (True Negative): correct negative prediction; FN (False Negative): incorrect negative prediction.

Table: Quantitative measure of performance for different classifiers.

Classifier	Precision	Recall	F-measure	Accuracy (%)
LR	0.964	0.794	0.871	77.143
LDA	0.964	0.794	0.871	77.143
kNN	0.800	1.000	0.889	80.000
SVM	0.964	0.771	0.857	75.000
RF	0.823	1.000	0.903	82.857
CART	0.823	1.000	0.903	83.333
ANN	0.928	0.812	0.867	77.142
Neural Trees	0.918	0.894	0.906	85.169
Entropy Nets	0.839	0.928	0.881	80.555
Proposed Ensemble CT-ANN	**0.942**	**0.970**	**0.956**	**91.667**

Other Applications: Medical Data Sets

Data Sets: The proposed model is evaluated using six publicly available medical data sets from Kaggle (https://www.kaggle.com/datasets) and UCI Machine Learning repository (https://archive.ics.uci.edu/ml/datasets.html) dealing with various diseases. These binary classification data sets have limited number of observations and high-dimensional feature spaces.

Table: Characteristics of the data sets used in experimental evaluation

Data set	Classes	Objects (n)	Number of feature (p)	Number of (+)ve instances	Number of (−)ve instances
breast cancer	2	286	9	85	201
heart disease	2	270	13	120	150
pima diabetes	2	768	8	500	268
promoter gene sequences	2	106	57	53	53
SPECT heart images	2	267	22	55	212
wisconsin breast cancer	2	699	9	458	241

Experimental Results

Table: Results (and their standard deviation) of classification algorithms over 6 medical data sets

Classifiers	Data set	The number of (reduced) features after feature selection	Classification accuracy (%)	F-measure
CT	breast cancer	7	68.26 (6.40)	0.70 (0.07)
	heart disease	7	76.50 (4.50)	0.81 (0.03)
	pima diabetes	6	71.85 (4.94)	0.74 (0.03)
	promoter gene sequences	17	69.43 (2.78)	0.73 (0.01)
	SPECT heart images	9	75.70 (1.56)	0.78 (0.00)
	wisconsin breast cancer	8	94.20 (2.98)	0.89 (0.01)
ANN (with 1HL)	breast cancer	9	61.58 (5.89)	0.64 (0.04)
	heart disease	13	73.56 (5.44)	0.79 (0.02)
	pima diabetes	8	66.78 (4.58)	0.69 (0.04)
	promoter gene sequences	57	61.77 (3.46)	0.65 (0.02)
	SPECT heart images	22	79.69 (0.23)	0.81 (0.01)
	wisconsin breast cancer	9	94.80 (2.01)	0.96 (0.01)
Entropy Nets	breast cancer	7	69.00 (6.25)	0.72 (0.05)
	heart disease	7	79.59 (4.78)	0.83 (0.01)
	pima diabetes	6	69.50 (4.05)	0.72 (0.02)
	promoter gene sequences	17	66.23 (1.98)	0.70 (0.01)
	SPECT heart images	9	76.64 (1.70)	0.78 (0.01)
	wisconsin breast cancer	8	95.96 (2.18)	0.96 (0.00)
DNDT	breast cancer	8	66.12 (7.81)	0.68 (0.08)
	heart disease	7	81.05 (3.89)	0.86 (0.02)
	pima diabetes	6	69.21 (5.08)	0.72 (0.05)
	promoter gene sequences	17	69.06 (1.75)	0.71 (0.01)
	SPECT heart images	10	75.50 (0.89)	0.77 (0.00)
	wisconsin breast cancer	7	94.25 (2.14)	0.95 (0.00)
Proposed Model	breast cancer	7	**72.80** (6.54)	**0.77** (0.06)
	heart disease	7	**82.78** (4.78)	**0.89** (0.02)
	pima diabetes	6	**76.10** (4.45)	**0.79** (0.04)
	promoter gene sequences	17	**75.40** (1.50)	**0.79** (0.01)
	SPECT heart images	9	**81.03** (0.56)	**0.82** (0.00)
	wisconsin breast cancer	8	**97.30** (1.05)	**0.98** (0.00)

Simulation Study

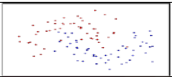
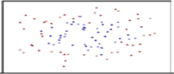
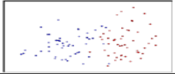
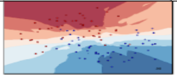
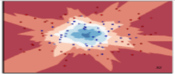
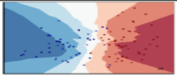
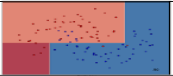
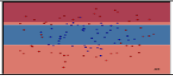
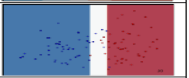
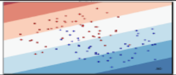
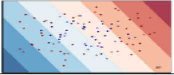
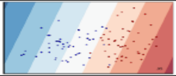
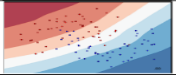
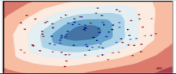
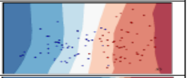
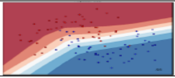
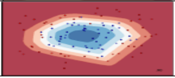
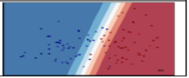
Simulated Data Sets: Three popularly used toy data sets (number of samples to be 100) are generated to visualize the decision boundaries of the classification algorithms used in this chapter. In all the experiments, 60% of the data samples are used for training, and the rest 40% of the data are for testing. The details of the data generation process are described with codes here: `https://github.com/scikit-learn/scikit-learn/blob/0fb307bf3/sklearn/datasets/_samples_generator.py`.

Table: Classification accuracy percentage of different classifiers on three synthetic data sets. Best results in the Table are made **bold**.

Classifiers	Moon data	Circle data	Linearly-separable data
kNN	90	82	90
CT	90	68	93
Linear SVM	90	40	95
ANN	88	60	93
Hybrid CT-ANN	**93**	**90**	**95**

Simulation Study

A comparison of several classifiers on synthetic data sets. The plots show training points in solid colors and testing points semi-transparent. The lower right in each plot shows the classification accuracy on the test set.

Synthetic data Classifiers	Moon data set	Circle data set	Linearly-separable data set
Input Data			
kNN			
CT			
Linear SVM			
ANN			
Hybrid CT-ANN			

Conclusions

- A novel nonparametric ensemble classifier is proposed to achieve higher accuracy in classification performance with very little computational cost (by working with a subset of input features).
- Our proposed feature selection cum classification model is robust in nature.
- Ensemble CT-ANN is shown to be universally consistent and less time consuming during the actual implementation.
- We have also found the optimal value of the number of neurons in the hidden layer so that the user will have less tuning parameters to be controlled.
- But many Real-world data sets are usually skewed, in that many cases belong a larger class and fewer cases belong to a smaller yet usually more exciting class.
- In the next chapter, we are going to consider the problem of data imbalanced in classification framework.

CHAPTER 4: HELLINGER NET: A HYBRID MODEL FOR IMBALANCED LEARNING

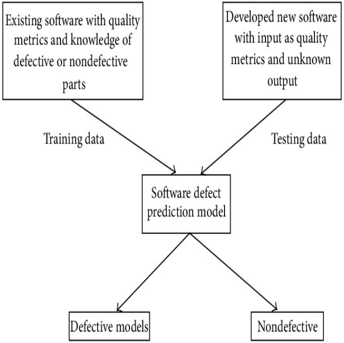
Publications:

1. Tanujit Chakraborty and Ashis Kumar Chakraborty. “Hellinger Net: A Hybrid Imbalance Learning Model to Improve Software Defect Prediction”. **IEEE Transactions on Reliability** (2020). **(Read Online)**

2. Tanujit Chakraborty and Ashis Kumar Chakraborty. “Superensemble Classifier for Improving Predictions in Imbalanced Datasets”, **Communications in Statistics: Case Studies, Data Analysis and Applications**, 6 (2020): 123-141. **(Read Online)**

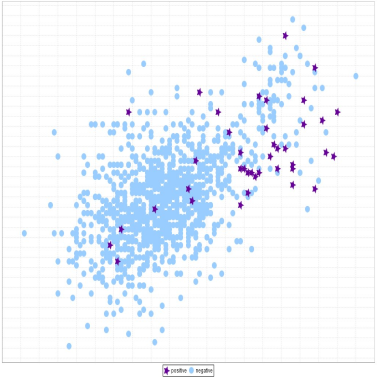
Motivation

- Software defect prediction is important to identify defects in the early phases of software development life cycle.
- This early identification and thereby removal of software defects is crucial to yield a cost-effective and good quality software product.
- Though, previous studies have successfully used machine learning techniques for software defect prediction, these techniques yield biased results when applied on imbalanced data sets.
- This study proposes an ensemble classifier, namely Hellinger Net, for software defect prediction on imbalanced NASA data sets.


Existing software with quality metrics and knowledge of defective or nondefective parts
Developed new software with input as quality metrics and unknown output
Training data
Testing data
Software defect prediction model
Defective models
Nondefective

Imbalanced Classification Problem

- Real-world data sets are usually skewed, in that many cases belong a larger class and fewer cases belong to a smaller yet usually more exciting class
- For example, consider a binary classification problem with the class distribution of 90 : 10. In this case, a straightforward method of guessing all instances to be positive class would achieve an accuracy of 90%.
- Learning from an imbalanced data set presents a tricky problem in which traditional learning algorithms perform poorly.
- Traditional classifiers usually aim to optimize the overall accuracy without considering the relative distribution of each class.



Sampling Techniques

- One way to deal with the imbalanced data problems is to modify the class distributions in the training data by applying sampling techniques to the data set
- Sampling technique either oversamples the minority class to match the size of the majority class or undersamples the majority class to match the size of the minority class.
- Synthetic minority oversampling technique (SMOTE) is among the most popular methods that oversamples the minority class by generating artificially interpolated data (Chawla et al., 2002, JAIR).
- TL (Tomek links) and ENN (edited nearest neighbor) are popular undersampling approaches (Batista et al., 2004, ACM SIGKDD).
- But these approaches have apparent deficiencies, such as undersampling majority instances may lose potentially useful information of the data set and oversampling increases the size of the training data set which may increase computational cost.
- To overcome these problems, “imbalanced data-oriented” algorithms are designed which can handle class imbalance without any modification to class distribution.

Effect of Class Imbalance on Decision Tree

Let X be attribute and Y be the response class. Here Y^{+} denotes majority class, Y^{-} denotes minority class and n is the total number of instances. Also, let $X^{\geq} \longrightarrow Y^{+}$ and $X^{<} \longrightarrow Y^{-}$ be two rules generated by CT. Table below shows the number of instances based on the rules created using CT.

Table: An example of notions of classification rules

class and attribute	$X^{\geq}$	$X^{<}$	sum of instances
Y^{+}	a	b	$a+b$
Y^{-}	c	d	$c+d$
sum of attributes	$a+c$	$b+d$	n

In the case of imbalanced data set the majority class is always much larger than the size of the minority class and thus we will always have $a+b >> c+d$. It is clear that the generation of rules based on confidence in CT is biased towards majority class.

Various measures, like information gain (IG), gini index (GI) and misclassification impurity (MI) expressed as a function of confidence, are used to decide which variable to split in the important feature selection stage, get affected by class imbalance.

Effect of Class Imbalance on Distance Measures

Table: An example of notions of classification rules

class and attribute	$X^{\geq}$	$X^{<}$	sum of instances
Y^{+}	a	b	$a+b$
Y^{-}	c	d	$c+d$
sum of attributes	$a+c$	$b+d$	n

Using Table 1, we compute the following:

$$P(Y^{+}/X^{\geq}) = \frac{a}{a+c} = \text{Confidence}(X^{\geq} \longrightarrow Y^{+})$$

For an imbalanced data set, Y^{+} will occur more frequently with $X^{\geq}$ & $X^{<}$ than to Y^{-}. So the concept of confidence is a fatal error in an imbalanced classification problem.

Entropy at node t is defined as:

$$\text{Entropy}(t) = -\sum_{j=1,2} P(j/t) log\big(P(j/t)\big)$$

Effect of Class Imbalance on Distance Measures

In binary classification, information gain for splitting a node t is defined as:

$$\mathrm{IG} = \mathrm{Entropy}(t) - \sum_{i=1,2} \frac{n_i}{n} \mathrm{Entropy}(i) \tag{0.6}$$

where i represents one of the sub-nodes after splitting (assuming we have two sub nodes only), n_i is the number of instances in sub-node i and n is the total number of instances. The objective of classification using CT is to maximize IG which reduces to:

$$\text{Maximize}\left\{ - \sum_{i=1,2} \frac{n_i}{n} \mathrm{Entropy}(i) \right\} \tag{0.7}$$

The maximization problem in eqn. (1.7) reduces to:

$$\begin{aligned}\text{Maximize}\Bigg\{ & \frac{n_1}{n}\Big[P(Y^+/X^{\geq}) log\big(P(Y^+/X^{\geq})\big) + P(Y^-/X^{\geq}) log\big(P(Y^-/X^{\geq})\big)\Big] \\ & + \frac{n_2}{n}\big[P(Y^+/X^{<}) log\big(P(Y^+/X^{<})\big) + P(Y^-/X^{<}) log\big(P(Y^-/X^{<})\big)\big]\Bigg\}\end{aligned} \tag{0.8}$$

The task of selecting the "best" set of features for node i are carried out by picking up the feature with maximum IG. As $P(Y^+/X^{\geq}) >> P(Y^-/X^{\geq})$, we face a problem while maximizing eqn. (0.8).

Hellinger Distance

Let (Θ, λ) denote a measurable space. Let us suppose that P and Q be two continuous distributions with respect to the parameter λ having the densities p and q in a continuous space Ω, respectively. Define HD as follows:

$$d_H(P,Q) = \sqrt{\int_\Omega (\sqrt{p} - \sqrt{q})^2 d\lambda} = \sqrt{2\left(1 - \int_\Omega \sqrt{pq} d\lambda\right)}$$

where $\int_\Omega \sqrt{pq} d\lambda$ is the Hellinger integral. It is noted that HD doesn't depend on the choice of the parameter λ.

For the application of HD as a decision tree criterion, the final formulation can be written as follows:

$$HD = d_H(X_+, X_-) = \sqrt{\sum_{j=1}^{k} \left(\sqrt{\frac{|X_{+j}|}{|X_+|}} - \sqrt{\frac{|X_{-j}|}{|X_-|}}\right)^2}, \qquad (0.9)$$

where $|X_+|$ indicates the number of examples that belong to the majority class in training set and $|X_{+j}|$ is the subset of training set with the majority class and the value j for the feature X. The bigger the value of HD, the better is the discrimination between the features (Hellinger Distance Decision Tree, Chawla et al. 2008, ECML).

Proposed Model: Hellinger Net

- Hellinger Net is composed of three basic steps:

  (a) Converting a DT into rules (HD is used as criterion);
  (b) Constructing a two hidden layered NN from the rules;
  (c) Training the MLP using gradient descent backpropagation (Rumelhart, Hinton (1988).

- In decision trees, the overfitting occurs when the size of the tree is too large compared to the number of training data.

- Instead of using pruning methods (removing child nodes), HN employs a backpropagation NN to give weights to nodes according to their significance.

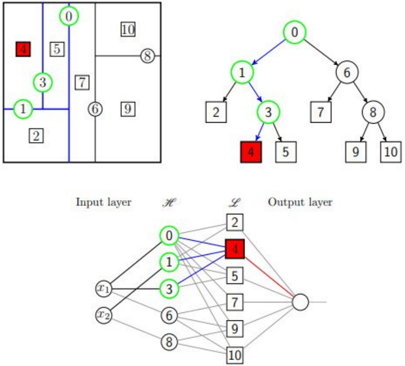


Fig: Graphical Representation of Hellinger Nets

The idea of the this approach is inspired from the idea of Perceptron Trees [Paul E Utgoff, 1988, AAAI]

Hellinger Net Algorithm

- Build a HDDT with $(k_n - 1)$ split nodes and k_n leaf nodes. HDDT is mapped into a two hidden layered MLP model having $(k_n - 1)$ and k_n hidden neurons in first hidden layer $(HL1)$ and second hidden layer $(HL2)$, respectively.
- The first hidden layer is called the partitioning layer which partitions the input feature spaces into different regions. It corresponds to the internal nodes of the DT. In $HL1$, the neurons compute all the tree split decisions and indicate the split directions for the inputs.
- Further, $HL1$ passes the information to $HL2$. The neurons in the second hidden layer represent the terminal nodes of the DT.
- The final layer is the output class label of the tree. Train the tree structured neural network using gradient descent backpropagation algorithm.
- Hellinger Net uses sigmoidal activation function instead of the relay-type activation function $\tau(u)$ with a hyperbolic tangent activation function $\sigma(u) = \tanh(u)$ which has a chosen range from -1 to 1.
- More precisely, the model uses $\sigma_1(u) = \sigma(\beta_1 u)$ at every neuron of the first hidden layer for better generalization, where β_1 is a positive hyper-parameter that determines the contrast of the hyperbolic tangent activation function.

Merits & Possible Extensions

- **Merits**:

  1. The additional training using backpropagation potentially improves the predictions of the HDDT and can deny tree pruning steps vis-a-vis the risk of overfitting.;

  2. Hellinger Nets give weight to nodes according to their significance as determined by the gradient backpropagation algorithm.;

  3. In Hellinger Nets, the neural network follows the built-in hierarchy of the originating tree since connections do not exist between all pairs of neurons in any two adjacent layers.;

  4. Since the number of neurons in the hidden layers are fixed, thus the training time is less.

- **Possible Extensions**:

  1. Theoretical Consistency?

  2. Rate of Convergence?

On Theoretical Consistency

Theorem (Chakraborty et al., 2020, IEEE Transactions on Reliability)

Assume X is uniformly distributed in $[0,1]^p$ and $Y = \{0,1\}$. As $n \to \infty$ and for any $k_n, \beta_1, \beta_2 \to \infty$ if the following conditions are satisfied:

$$
\begin{aligned}
&(A1) \quad \frac{k_n^4 log(\beta_2 k_n^4)}{n} \to 0,\\
&(A2) \quad \textit{there exists} \quad \delta > 0 \quad \textit{such that} \quad \frac{k_n^2}{n^{1-\delta}} \to 0,\\
&(A3) \quad \frac{k_n^2}{e^{2\beta_2}} \to 0, \quad \textit{and}\\
&(A4) \quad \frac{k_n^3 \beta_2}{\beta_1} \to 0,
\end{aligned}
$$

then Hellinger Nets classifier is consistent.

The above Theorem states that with certain restrictions imposed on the number k_n of terminal nodes and the parameters β_1, β_2 being properly regulated as functions of n, the empirical L_1 risk-minimization provides local consistency of the Hellinger Nets classifier.

Rate of Convergence

Theorem (Chakraborty et al., 2020, IEEE Transactions on Reliability)

Assume that X is uniformly distributed in $[0,1]^p$ and $Y = \{0,1\}$ and a function $m : C^p \to \{0,1\}$ satisfies $|m(x) - m(z)| \leq c\|x-z\|^{\delta}$ for any $\delta \in [0,1]$ and $z \in [0,1]^p$. Let m_n be the estimate that minimizes empirical L_1-risk and the network activation function σ_i satisfies Lipschitz property. Then for any $n \geq max\{\beta_2, 2^{p+1}L\}$, we have

$$E \int_{[0,1]^p} \left|m_n(X) - m(X)\right| \mu(dx) = O\left(\frac{log(n)^6}{n}\right)$$

- The proof of the Theorem is using Complexity Regularization Principles.
- The rate of convergence doesn't depend on the data dimension and hence the model will be able to circumvent the so-called problem of "curse of dimensionality".
- In practice, the larger the value of k_n, β_1, and β_2, the better the model performance is.

Applications: Data Sets

Data Sets: The proposed model is evaluated using five publicly available data sets from the area of Software Defect Prediction (NASA Metrics Data Program) available at Promise Software Engineering repository (`http://promise.site.uottawa.ca/SERepository/datasets-page.html`).

Table: Characteristics of the data sets used in experimental evaluation

Data set	Classes	Objects (n)	Number of feature (p)	Number of reported defects	Number of non-defects
CM1	2	498	21	49	449
JM1	2	10885	21	2106	8779
KC1	2	2109	21	326	1783
KC2	2	522	21	105	415
PC1	2	1109	21	77	1032

Performance Evaluation

The performance evaluation measure used in our experimental analysis is based on the confusion matrix in Table 2. Area under the receiver operating characteristic curve (AUC) is a popular metric for evaluating performances of imbalanced data sets and higher the value of AUC, the better the classifier is. AUC $= \frac{\text{Sensitivity}+\text{Specificity}}{2}$; where, Sensitivity $= \frac{TP}{TP+FN}$; Specificity $= \frac{TN}{FP+TN}$.

Table: Average AUC value for balanced data sets (using SMOTE and SMOTE+ENN) on different classifiers

Data	Sampling Techniques	kNN	CT	RF	ANN (with 1HL)	ANN (with 2HL)	RBFN
CM1	SMOTE	0.700	0.665	**0.722**	0.605	0.680	0.704
	SMOTE+ENN	0.685	0.650	0.708	0.600	0.652	0.700
JM1	SMOTE	0.758	0.745	0.762	0.740	0.735	0.764
	SMOTE+ENN	0.760	**0.778**	0.770	0.750	0.720	0.765
KC1	SMOTE	0.783	0.845	0.859	0.765	0.798	0.905
	SMOTE+ENN	0.801	0.850	0.875	0.798	0.807	**0.914**
KC2	SMOTE	0.927	0.965	**0.967**	0.933	0.942	0.954
	SMOTE+ENN	0.935	0.952	0.966	0.925	0.937	0.949
PC1	SMOTE	0.770	0.758	0.753	0.698	0.719	0.745
	SMOTE+ENN	**0.788**	0.760	0.761	0.712	0.725	0.748

Performance Evaluation

Highest AUC value in both the tables are highlighted with dark black for all the data sets. It is clear from computational experiments that our model stands as very much competitive with the current state-of-the-art models.

Table: AUC results (and their standard deviation) of classification algorithms over original imbalanced test data sets

Classifiers	CM1	JM1	KC1	KC2	PC1
CT	0.603 (0.04)	0.665 (0.03)	0.810 (0.04)	0.950 (0.00)	0.724 (0.02)
RF	0.690 (0.06)	0.725 (0.03)	0.850 (0.04)	0.964 (0.00)	0.747 (0.04)
k-NN	0.651 (0.03)	0.727 (0.01)	0.750 (0.03)	0.902 (0.02)	0.730 (0.05)
RBFN	0.652 (0.06)	0.723 (0.04)	0.884 (0.05)	0.935 (0.01)	0.725 (0.04)
HDDT	0.625 (0.04)	0.738 (0.04)	0.933 (0.02)	0.974 (0.00)	0.760 (0.02)
HDRF	0.636 (0.04)	0.742 (0.03)	0.939 (0.02)	**0.988** (0.00)	0.760 (0.03)
CCPDT	0.618 (0.05)	0.712 (0.05)	0.912 (0.03)	0.971 (0.00)	0.753 (0.01)
ANN (with 1HL)	0.585 (0.03)	0.700 (0.03)	0.768 (0.05)	0.918 (0.02)	0.649 (0.03)
ANN (with 2HL)	0.621 (0.02)	0.715 (0.02)	0.820 (0.04)	0.925 (0.01)	0.710 (0.03)
Hellinger Net	**0.720** (0.06)	**0.798** (0.04)	**0.964** (0.01)	0.985 (0.00)	**0.789** (0.05)

Simulation Study

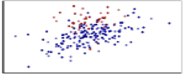
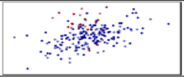
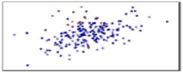
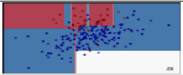
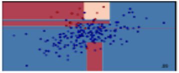
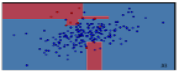
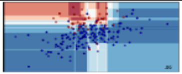
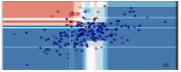
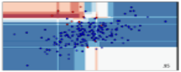
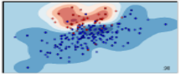
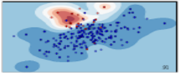
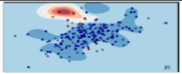
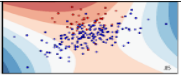
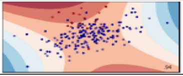
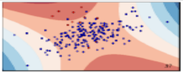
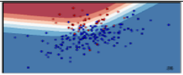
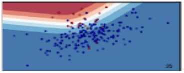
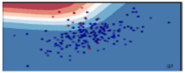
Simulated Data Sets: Three toy data sets (binary) are generated with weights = [0.2, 0.8], [0.1, 0.9] and [0.05, 0.95], i.e., data sets with imbalance rates of 20%, 10% and 5%, respectively. We added Gaussian noise to the data with the standard deviation equals to 0.5. This test problem is suitable for algorithms that can learn data imbalance problems in complex nonlinear manifolds.

Table: AUC results of different imbalanced classifiers on three synthetic data sets.

Imbalanced Classifiers	Simulated Data with IR = 20%	Simulated Data with IR = 10%	Simulated Data with IR = 5%
HDDT	0.80	0.85	0.91
HDRF	0.82	0.88	0.91
VCB-SVM	**0.87**	0.89	0.93
ISDA	0.84	0.91	0.90
Hellinger net	0.86	**0.92**	**0.95**

Simulation Study

A comparison of several imbalanced classifiers on synthetic data sets. The plots show training points in solid colors and testing points semi-transparent. The lower right in each plots shows the classification accuracy on the test set.

Synthetic data	Imbalance = 20% rate	Imbalance = 10% rate	Imbalance = 5% rate
Input Data			
HDDT			
HDRF			
VCB-SVM			
ISDA			
Hellinger net			

Conclusions

- Learning from an imbalanced data set presents a tricky problem in which traditional learning models perform poorly.
- Simply allocating half of the training examples to the minority class does not provide the optimal solution in most of the real-life problems.
- If one would like to work with the original data without taking recourse to sampling, our proposed hybrid methodology will be quite handy.
- We proposed ‘Hellinger Nets’, a hybrid learner, that first construct a tree and then simulate it using neural networks.
- We also show the consistency and rate of convergence of Hellinger Nets algorithm.
- In the next chapter, we are going to consider another common problem of predictive analytics, namely regression.

Chapter 5: A Distribution-free Hybrid Method for Regression Modeling

Publications:

1. Tanujit Chakraborty, Ashis Kumar Chakraborty, and Swarup Chattopadhyay. "A novel distribution-free hybrid regression model for manufacturing process efficiency improvement", **Journal of Computational and Applied Mathematics**, 362 (2019): 130-142. **(Read Online)**

2. Tanujit Chakraborty, Swarup Chattopadhyay, and Ashis Kumar Chakraborty. "Radial basis neural tree model for improving waste recovery process in a paper industry", **Applied Stochastic Models in Business and Industry**, 36 (2020): 49-61. **(Read Online)**

Motivation

- This work is motivated by a particular problem in a modern paper manufacturing industry, in which maximum efficiency of the process fiber-filler recovery equipment, also known as Krofta supracell, is desired.

- As a by-product of the paper manufacturing process, a lot of unwanted materials along with valuable fibers and fillers come out as waste materials.

- The job of an efficient Krofta supracell is to separate the unwanted materials from the valuable ones so that fibers and fillers can be reused in the manufacturing process.

Fig: Krofta supracell

Process Efficiency Improvement Problem

- The Krofta recovery percentage was around 75%. The paper manufacturing company wants to improve the recovery percentage to 90%.

- To identify the important parameters affecting the Krofta efficiency, a failure mode and effect analysis (FMEA) was performed with the help of process experts.

- **Goal**: We would like to come up with a model that can help the manufacturing process industry to achieve an efficiency level of about 90% from the existing level of about 75% to improve the Krofta supracell recovery percentage.

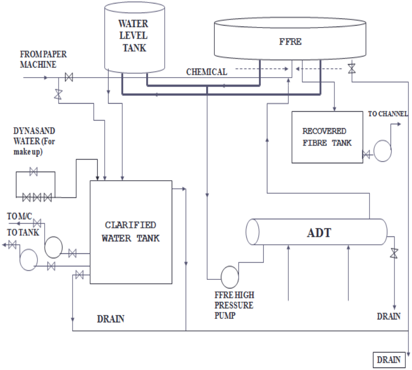


Fig: Process Flow Diagram of Krofta supracell

Process Data Set

- The data set collected for a year from the process on the following causal variables: Inlet Flow, Water Pressure (water inlet pressure to ADT), Air Pressure, Pressure of Air-Left, Pressure of Air-Right, Pressure of ADT-D Left, Pressure of ADT-D Right and Amount of chemical lubricants.
- The response variable (FFRE recovery percentage) lies between 20 to 100.
- This data set will be used for finding crucial process parameters and also finding a prediction model that can help the company for forecasting future recovery percentage of FFRE.

Table: Sample data set

Inlet Flow	Water Pressure	Air Pressure	Air-Left	Air-Right	ADT-D	ADT-D	Amount of	Recovery
						Left	Right	chemical
Percentage								
1448	6.4	5.8	1.0	2.1	3.2	4.0	2.0	96.80
1794	5.2	5.6	2.4	1.6	3.6	4.0	3.0	97.47
2995	6.0	6.0	1.5	4.5	4.0	4.8	4.0	28.87
1139	6.5	6.0	1.2	1.7	3.0	4.6	2.0	33.05
2899	6.2	5.7	2.0	1.2	3.1	4.0	2.0	97.91
1472	6.6	6.8	3.7	3.1	5.2	4.8	4.0	57.77
1703	6.2	6.0	2.9	1.0	3.0	4.2	2.0	26.94
1514	5.5	5.0	2.0	2.1	3.8	4.7	2.0	67.01
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.

Proposed Hybrid RBNT Model

- Apply RT algorithm to train and build a decision tree. Use the tree to extract the important features and find the splits between different adjacent values of the features.
- Choose the features that have minimum mean squared error as important input variables and record RT predicted outputs.
- Export important input variables along with an additional feature (prediction values of RT algorithm) to the RBFN model and a neural network is generated.
- RBFN model uses Gaussian kernel as an activation function, and parameter optimization is done using gradient descent algorithm. Finally, we obtain the final outputs.

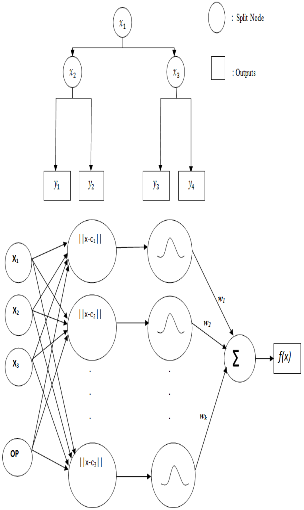


Fig: Flowchart of the Proposed Radial Basis Neural Tree Model

Theoretical Consistency

Theorem (Chakraborty et al., 2020, Applied Stochastic Models)

Suppose $(\underline{X}, \underline{Y})$ be a random vector in $\mathbb{R}^p \times [-K, K]$ and L_n be the training set of n outcomes of $(\underline{X}, \underline{Y})$. Finally if for every n and $w_i \in \tilde{\Omega}_n$, the induced subset $(L_n)_{w_i}$ contains at least k_n of the vectors of $X_1, X_2, ..., X_n$, then empirically optimal regression trees strategy employing axis parallel splits are consistent when the size k_n of the tree grows as $o(\frac{n}{log(n)})$.

Theorem (Chakraborty et al., 2020, Applied Stochastic Models)

Consider a RBF network with Gaussian radial basis kernel having one hidden layer with k (> 1) nodes. If $k \to \infty$, $b \to \infty$ and $\frac{kb^4 log(kb^2)}{n} \to 0$ as $n \to \infty$, then RBFN model is said to be universally consistent for all distribution of $(\underline{Z}, \underline{Y})$.

On the choice of Number of Hidden Neurons

- RBFN is a family of ANNs, consists of only a single hidden layer and uses radial basis function as an activation function, unlike feed forward neural network. RBF network with one hidden layer having k nodes for a fixed Gaussian function is given by the equation:

$$f(z_i) = \sum_{j=1}^{k} w_j \; exp\left(- \frac{\| \; z_i - c_i \; \|^2}{2\sigma_i^2} \right) + w_0,$$

  where $\sum_{j=0}^{k} |w_j| \leq b \; (> 0)$ and $c_1, c_2, ..., c_k \in \mathbb{R}^{d_m}$.

- For practical use, if the data set is limited, the recommendation is to use $k = \left(\sqrt{n/d_m log(n)}\right)$ for achieving utmost accuracy of the propose model.

Proposition (Chakraborty et al., 2019, Journal of Comp. & Appl. Mathematics)

For any fixed d_m and training sequence ξ_n, let $Y \in [-K, K]$, and $m, f \in F_{n,k}$, if the neural network estimate m_n satisfies the above-mentioned regularity conditions of strong universal consistency and f satisfying $\int_{S_r} f^2(z)\mu(dz) < \infty$ where, S_r is a ball with radius r centered at 0, then the optimal choice of k is $O\left(\sqrt{\frac{n}{d_m log(n)}}\right)$.

Experimental Evaluation

Popularly used performance metric are:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \widehat{y}_i\right|;\ RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y}_i)^2};\ MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \widehat{y}_i}{y_i}\right|;$$

$$R^2 = 1 - \left[\frac{\sum_{i=1}^{n}(y_i - \widehat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \overline{y})^2}\right];\ AdjR^2 = 1 - \left[\frac{(1-R^2)(n-1)}{n-d_m-1}\right];$$

where, $y_i, \overline{y}, \widehat{y}_i$ denote the actual value, average value and predicted value of the dependent variable, respectively for the i^{th} instant. Here n and d_m denote the number of data points and independent variables used for performance evaluation, respectively.

Table: Quantitative measure of performance for different regression models. Results are based on 10 fold cross validations. Mean values of the respective measures are reported with standard deviation within the bracket.

Models	**MAE**	**RMSE**	**MAPE**	R^2	**Adj(R^2)**
RT	11.691 (0.45)	16.927 (0.89)	29.010 (1.02)	59.028 (3.25)	55.304 (1.95)
ANN	12.334 (0.25)	17.073 (0.56)	27.564 (1.85)	58.310 (2.98)	54.529 (2.08)
SVR	12.460 (0.28)	20.362 (1.23)	40.010 (1.81)	40.174 (2.05)	35.325 (2.64)
BART	12.892 (0.59)	16.010 (1.25)	30.038 (1.95)	59.380 (2.50)	56.458 (1.75)
RBFN	13.926 (2.50)	18.757 (3.25)	32.48 (3.45)	49.689 (5.45)	46.335 (3.95)
Tsai Neural tree	10.895 (0.78)	16.012 (0.50)	24.021 (1.85)	65.120 (2.89)	62.946 (1.78)
Proposed Model	**9.226** (0.35)	**14.331** (0.82)	**20.187** (1.45)	**70.632** (2.00)	**68.675** (2.13)

Other Experiments

Data Sets: The proposed model is evaluated using six publicly available from UCI Machine Learning repository (`https://archive.ics.uci.edu/ml/datasets.html`). These regression data sets have limited number of observations.

Table: Data set characteristics: number of samples and number of features, after removing observations with missing information or nonnumerical input features.

Sl. No.	Data	Number of samples	Number of features
1	Auto MPG	398	7
2	Concrete	1030	8
3	Forest Fires	517	10
4	Housing	506	13
5	Wisconsin	194	32

Table: Average RMSE results for each of the models across the different data sets

Data	RT	ANN	SVR	BART	RBFN	Neural Tree	Our Model
Auto MPG	3.950	4.260	5.720	3.220	4.595	3.300	**3.215**
Concrete	8.700	10.180	11.588	**5.540**	10.210	7.420	7.063
Forest Fires	75.138	90.702	91.985	65.890	82.804	**62.478**	64.411
Housing	4.980	9.054	12.520	3.978	7.871	4.590	**3.077**
Wisconsin	41.059	34.710	41.220	32.054	38.495	40.700	**23.659**

Application to Simulated data

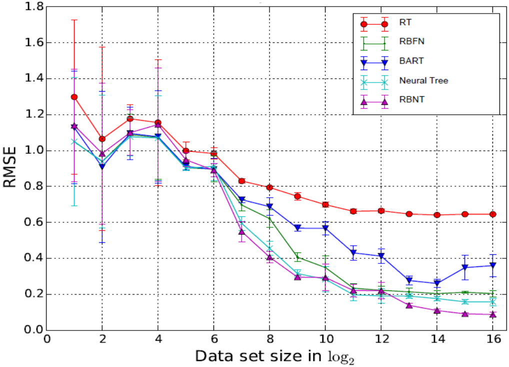
We investigate the asymptotic behavior of the proposed RBNT model on an artificial data set created by sampling inputs $\underline{x}$ uniformly from the p-dimensional hypercube $[0,1]^p$ and computing outputs y as

$$y(x) = \sum_{j=1}^{p} \sin\left(20x^{(j)} - 10\right) + \varepsilon,$$

where ε is a zero mean Gaussian noise with variance σ^2, which corrupts the deterministic signal. We choose $p = 2$ and $\sigma = 0.01$, and investigate the asymptotic behavior as the number of training samples increases. Figure in the next slide illustrates the RMSE for an increasing number of training samples and shows that the RBNT model error decreases much faster than other competitive model errors as sample size increases.

Asymptotic Behavior

This figure shows the test RMSE for synthetic data with exponentially increasing training set size (x-axis). Solid lines connect the mean RMSE values obtained across 3 randomly drawn data sets for each data set size, whereas error bars show the empirical standard deviation.



Conclusions

- In this chapter, we build a hybrid regression model for improving the process efficiency in a paper manufacturing company.
- Our study presented a hybrid RT-RBFN model that integrates RT and RBFN algorithm which gives more accuracy than all other competitive models to address the Krofta efficiency improvement problem.
- The proposed model is consistent, and when applied to other complex regression problems, it performed well as compared to other state-of-the-art.
- The usefulness and effectiveness of the model lie in its robustness and easy interpretability as compared to complex "black-box-like" models.

Chapter 6: Bayesian Neural Tree Models for Nonparametric Regression

Publications:

1. Tanujit Chakraborty, Ashis Kumar Chakraborty, and Zubia Mansoor. "A hybrid regression model for water quality prediction", **Opsearch**, 56 (2019): 1167-1178. **(Read Online)**

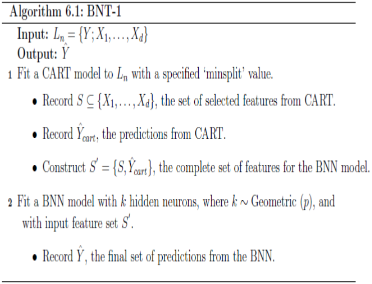
2. Tanujit Chakraborty, Gauri Kamat, and Ashis Kumar Chakraborty. "Bayesian neural tree models for nonparametric regression", Under Review. **(Read Online)**

Motivation

- Frequentist and Bayesian methods differ in many aspects but share some basic optimal properties. In real-life prediction problems, situations exist in which a model based on one of the above paradigm is preferable depending on some subjective criterion.
- Nonparametric classification and regression techniques, such as decision trees and neural networks, have frequentist (classification and regression trees (CART) and artificial neural networks) as well as Bayesian (Bayesian CART and Bayesian neural networks) approach to learning from data..
- In this chapter. we present two hybrid models combining the Bayesian and frequentist versions of CART and neural networks, which we call the Bayesian neural tree (BNT) model. BNT model can simultaneously perform feature selection and prediction, are highly flexible, and generalize well in settings with a limited number of training observations.

Bayesian Neural Tree-1 Model

- The BNT-1 model comprises of two stages. In the first stage, a classical CART model is fit to the data, taking all d predictors. The CART model implicitly selects a feature at each internal split (based on maximum reduction in the MSE).
- We record these features, as well as the predictions obtained from the CART model and use them in the second stage to construct a BNN with one hidden layer.
- We use a Gaussian prior for the network weights and also model the data likelihood to be Gaussian. The prior for the number of hidden neurons (k) is taken to be a Geometric distribution with probability of success p.
- Finally, we obtain the final outputs.



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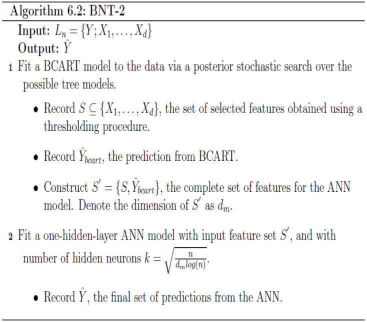
Algorithm 6.1: BNT-1
  Input: $L_n = \{Y; X_1, \ldots, X_d\}$
  Output: $\hat{Y}$
1 Fit a CART model to $L_n$ with a specified 'minsplit' value.
    • Record $S \subseteq \{X_1, \ldots, X_d\}$, the set of selected features from CART.
    • Record $\hat{Y}_{cart}$, the predictions from CART.
    • Construct $S' = \{S, \hat{Y}_{cart}\}$, the complete set of features for the BNN model.
2 Fit a BNN model with $k$ hidden neurons, where $k \sim$ Geometric $(p)$, and
  with input feature set $S'$.
    • Record $\hat{Y}$, the final set of predictions from the BNN.
```

Fig: Algorithm of the BNT-1 Model

Bayesian Neural Tree-2 Model

- The BNT-2 model also follows a two-step pipeline. A BCART model is fit to the data in the first stage, with the best fitting tree found via posterior stochastic search.
- We record the important features and predictions from BCART, and use these as inputs to a one-hidden-layer ANN in stage two.
- Export important input variables along with an additional feature (prediction values of BCART algorithm) to an optimal ANN model and a neural network is generated.
- Finally, we obtain the final outputs.



```
Algorithm 6.2: BNT-2
  Input: $L_n = \{Y; X_1, \ldots, X_d\}$
  Output: $\hat{Y}$
1 Fit a BCART model to the data via a posterior stochastic search over the
  possible tree models.
    • Record $S \subseteq \{X_1, \ldots, X_d\}$, the set of selected features obtained using a
      thresholding procedure.
    • Record $\hat{Y}_{bcart}$, the prediction from BCART.
    • Construct $S' = \{S, \hat{Y}_{bcart}\}$, the complete set of features for the ANN
      model. Denote the dimension of $S'$ as $d_m$.
2 Fit a one-hidden-layer ANN model with input feature set $S'$, and with
  number of hidden neurons $k = \sqrt{\frac{n}{d_m log(n)}}$.
    • Record $\hat{Y}$, the final set of predictions from the ANN.
```

Fig: Algorithm of the BNT-2 Model

Asymptotic Consistency for BNT-1 Model

Theorem (Chakraborty et al., 2019)

Assume that $\mathbb{Z}$ is uniformly distributed in $[0,1]^{d_m}$, $\Pi_i \overset{ind}{\sim} \mathcal{N}(0,\tau^2)$, $k \sim$ Geometric(p), and the following conditions hold:
(A1) For all i, we have $\lambda_i > 0$;
(A2) $B_n \uparrow n$, for all $r > 0$, there exists $q > 1$ and N such that $\sum_{i=B_n+1}^{\infty} \lambda_i < exp\big(-n^q r\big)$ for $n \geq N$;
(A3) There exists $r_i > 0, N_i$ such that $\Pi_n(F_n^c) < exp(-nr_i)$ for all $n \geq N_i$;
(A4) For all $\gamma, v > 0$, there exists I and M_i such that for any $i \geq I$, $\Pi_i(K_\gamma) \geq exp(-nv)$ for all $n \geq M_i$.
Then for all $\epsilon > 0$, the posterior is asymptotically consistent for f_0 over Hellinger neighborhoods and $P\big(H_\epsilon \,|(Z_1, Y_1), ..., (Z_n, Y_n)\big) \rightarrow 1$ in probability.
In other words, the posterior probability of any Hellinger neighborhood of f_0 converges to 1 in probability, where H_ϵ is the Hellinger neighborhoods, K_γ is the Kullback-Leibler neighborhood, and We denote the prior for f by $\Pi_n(\cdot)$.

Above Theorem shows that the posterior is consistent when the number of hidden neurons of the neural network (with Bayesian setting) is a parameter that can be estimated from the data. Thus, we can let the data derive the number of hidden nodes in the model and emphasize on model selection during practical implementation.

Asymptotic Consistency for BNT-2 Model

Theorem (Chakraborty et al., 2019)

Consider an ANN with a logistic sigmoidal activation function having one hidden layer with k (> 1) hidden nodes. If k and β_n are chosen to satisfy

$$k \to \infty,\ \beta_n \to \infty,\ \frac{k\beta_n^4 log(k\beta_n^2)}{n} \to 0$$

as $n \to \infty$, then the model is said to be consistent for all distributions of $(\mathbb{Z}, \mathbb{Y})$ with $\mathbb{E}|\mathbb{Y}|^2 < \infty$.

Proposition (Chakraborty et al., 2019)

Assume that $\mathbb{Z}$ is uniformly distributed in $\mathbb{C}^{d_m}$ and $\mathbb{Y}$ is bounded a.s. and m is Lipschitz (δ, c)-smooth. Under the assumptions of the above Theorem, with fixed d_m, and $m, f \in F_{n,k}$, also f satisfying $\int_{C^{d_m}} f^2(z)\mu(dz) < \infty$, we have $k = O\left(\sqrt{\frac{n}{d_m log(n)}}\right)$.

Application to Water Quality Prediction

- We consider a particular problem in a modern paper industry that produces papers for multiple uses. Paper machines produce papers by using pulp, fiber, filler, chemical lubricant, and a considerable amount of water.

- The boiler produces steam for power generation purposes and also helps to make pulp for paper production. The steam produced in the boiler is used for cooking wood chips (along with the cooking chemicals).

- The boiler stipulates the desired level of water quality to be received from the water treatment plant. In the plant, the process of demineralization (DM process) is applied for the removal of dissolved solids by the ion exchange process (IEP) that involves two stages of demineralization

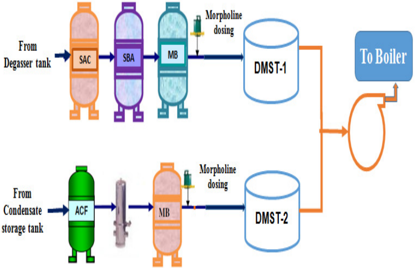


Fig: Process Flow Diagram of Krofta supracell

Process Data Set

- DM process outlet pH happens to be the key performance indicator (KPI) of the water treatment plant. It was found that the plant can not produce water of desired quality specified by the boiler to be supplied to the paper machine.
- Finding a prediction model for the water quality will help the company to address the problem of variation in DM outlet water pH as well as an indication for the health of the boiler water tube.
- An extensive preliminary data analysis was conducted to determine a set of possible causal variables that happen to be the key to water pH level variations.

Table: Sample data set for DMST-1

Sl. No.	Inlet Flow	Water Pressure	Air Pressure	MB stroke	Amount of chemical	DM water outlet pH
1	1980	5.8	5.0	70	9.96	9.276
2	2150	7.0	7.0	60	8.69	9.094
3	1780	6.0	5.0	45	7.73	8.594
4	2808	5.2	6.4	50	6.54	8.738
5	1590	6.2	5.7	40	5.56	8.592
6	2995	6.0	6.0	50	7.23	9.099
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.

Experimental Results

Table: Quantitative measures of performance for different regression models on test data set (average values of the metrics after 5-fold cross validations)

Regression Models	Data set	RMSE	MAPE	R^2	Adj R^2
Kernel SVR	DMST 1	4.06	4.50	75.66	70.29
	DMST 2	4.18	5.20	72.70	67.25
B-splines	DMST 1	4.32	5.40	69.85	63.30
	DMST 2	6.94	7.21	56.70	49.78
MARS	DMST 1	4.29	5.26	65.95	58.90
	DMST 2	6.74	7.93	57.53	47.05
RT	DMST 1	3.44	4.12	80.52	75.56
	DMST 2	3.89	4.78	76.56	71.23
ANN (with 2HL)	DMST 1	3.86	4.80	76.95	70.03
	DMST 2	4.12	5.91	70.10	64.73
BNT-2 Model	DMST 1	**3.05**	**3.40**	**85.40**	**82.50**
	DMST 2	**3.20**	**3.75**	**83.50**	**80.00**

Table: Optimal range of causal variables for achieving desired pH level

Process	Range for Water Pressure	Range for MB stroke	Range for chemical consumption	Expected range for DM water outlet pH
DMST 1	5.0-6.0	45-55	6.5-7.5	8.5-9.1
DMST 2	5.0-6.0	40-50	7.5-8.5	8.5-9.2

Conclusions

- In this work, we present two hybrid models that combine frequentist and Bayesian implementations of decision trees and neural networks.
- The proposed hybrid machine learning paradigm, when applied to solve water quality forecasting problems in a paper manufacturing industry, performs better than competing tools.
- An immediate extension of this work will be to develop hybrid methodology based on two Bayesian models, namely BCART and BNN to enhance uncertainty quantification and decision making in a fully nonparametric regression scenario.
- In the next chapter, we look at a different kind of regression problem, namely time series forecasting.

Chapter 7: A hybrid time series model for Macroeconomic forecasting

Publications:

Tanujit Chakraborty, Ashis Kumar Chakraborty, Munmun Biswas, Sayak Banerjee, and Shramana Bhattacharya. "Unemployment rate forecasting: A hybrid approach", **Computational Economics** (2020). **(Read Online)**

Linear Vs. Nonlinear Models in Time Series Forecasting

- Conventional statistical methods, the autoregressive integrated moving average (ARIMA) (Box and Jenkins, 1976) is extensively utilized in constructing a forecasting model.
- ARIMA cannot be utilized to produce an accurate model for forecasting nonlinear time series.
- Machine Learning algorithms have been successfully utilized to develop a nonlinear model for forecasting time series.
- Determining whether a linear or nonlinear model should be fitted to a real-world data set is difficult.
- The ARIMA model is used for prediction non-stationary time series when linearity between variables is supposed.
- However, in many practical situations supposing linearity is not valid.

Background: ARIMA Model

- The ARIMA model, introduced by Box and Jenkin, is a linear regression model indulged in tracking linear tendencies in stationary time series data.
- The model is expressed as ARIMA(p,d, q) where p, d, and q are integer parameter values that decide the structure of the model.
- More precisely, p and q are the order of the AR model and the MA model respectively, and parameter d is the level of differencing applied to the data.
- The mathematical expression of the ARIMA model is as follows:

$$y_t = \theta_0 + \phi_1 y_{t-1} + \phi_2 y_{t-2} + \cdots + \phi_p y_{t-p} + \varepsilon_t - \theta_1 \varepsilon_{t-1} - \theta_2 \varepsilon_{t-2} - \cdots - \theta_q \varepsilon_{t-q},$$

- where y_t is the actual value, ε_t is the random error at time t, ϕ_i and θ_j are the coefficients of the model.
- It is assumed that ε_{t-l} ($\varepsilon_{t-l} = y_{t-l} - \hat{y}_{t-l}$) has zero mean with constant variance, and satisfies the i.i.d condition.
- Three Steps: Model identification, Parameter Estimation, and Diagnostic Checking.

Background: NNAR Model

- Neural nets are based on simple mathematical models of the brain, used for sophisticated nonlinear forecasting.
- NNAR (Faraway and Chatfield, JRSS C, 1998) overcomes the problems of fitting ANN for time series data sets like the choice on the number of hidden neurons, and its black box nature.
- NNAR model is a nonlinear time series model which uses lagged values of the time series as inputs to the neural network.
- NNAR(p,k) is a feed-forward neural network having one hidden layer with p lagged inputs and k nodes in the hidden layer.
- Thus, NNAR model with one hidden layer with the following mathematical form:

$$\hat{x_t} = \phi_0 \left\{ w_{c_0} + \sum_h w_{h_0} \phi_h \left(w_{c_h} + \sum_i w_{i_h} x_{t-j_i} \right) \right\}$$

  where $\{w_{c_h}\}$ denotes the connecting weights and ϕ_i is the activation function.
- An NNAR(p,k) model uses p as the optimal number of lags (calculated based on the AIC value) for an AR(p) model and k is set to $k = [\frac{(p+1)}{2}]$ for non-seasonal data sets.

Motivation for Hybrid Techniques

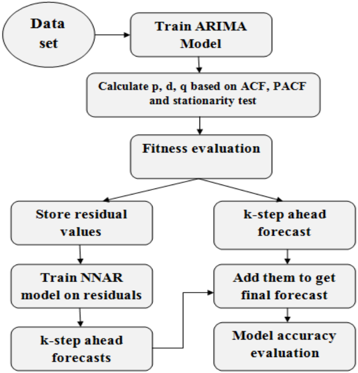
- A Forecaster wants the ARIMA model error series to be composed by i.i.d. random chocks or unpredictable or unsystematic terms with zero mean and constant variance, reflecting the piece of variability for which no reduction is possible.
- However, due to model mis-specification or to disturbances introduced in the stochastic process after forecasters elaboration, this (white noise) assumption may be violated during application phase.
- If the information underlying the error series is modeled, the performance of the original forecaster can be improved.

Table: Popular Hybrid Models in Time Series Forecasting Literature

Hybrid Model	**Author**	**Year**	**Journal**
SARIMA + BPNN	Tseng	2002	TFSC
ARIMA + ANN	Zhang	2003	Neurocomputing
ARIMA + SVM	Pai	2005	Omega
ARIMA + RNN	Aladag	2009	AML
ARIMA + PNN	Khashei	2012	C&IE
VARMA + BNN	Guo	2016	JAS
ARIMA + DNN	Qin	2017	KBS
Hybrid Survey	Khashei	2018	CinS

Proposed Additive Hybrid Model

- $Z_t = Y_t + N_t$, where Y_t is the linear part and N_t is the nonlinear part of the hybrid model.
- Both Y_t and N_t are estimated from the data set.
- Let, $\hat{Y}_t$ be the forecast value of the ARIMA model at time t and ε_t represent the residual at time t as obtained from the ARIMA model.
- Then $\varepsilon_t = Z_t - \hat{Y}_t$.
- The residuals are modeled by the NNAR model and can be represented as follows $\varepsilon_t = f(\varepsilon_{t-1}, \varepsilon_{t-2}, ..., \varepsilon_{t-n}) + \varsigma_t$, where f is a nonlinear function modeled by the NNAR approach and ς_t is the random error.
- Therefore, the combined forecast is $\hat{Z}_t = \hat{Y}_t + \hat{N}_t$, where, $\hat{N}_t$ is the forecast value of the NNAR model.



Data set
Train ARIMA Model
Calculate p, d, q based on ACF, PACF and stationarity test
Fitness evaluation
Store residual values
k-step ahead forecast
Train NNAR model on residuals
Add them to get final forecast
k-step ahead forecasts
Model accuracy evaluation

Fig: Graphical Representation of Hybrid ARIMA + NNAR Model

Applications: Unemployment Rate Data Sets

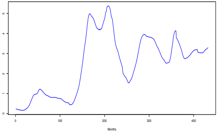
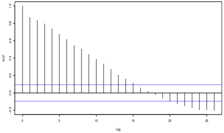
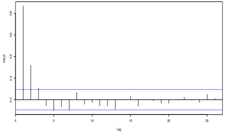
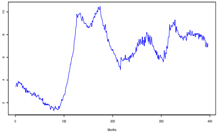
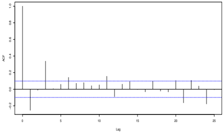
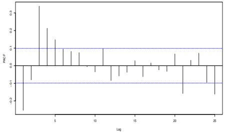
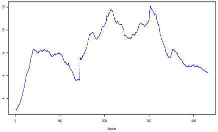
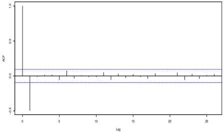
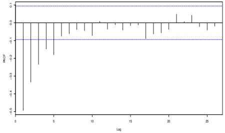
Region	Training data	ACF plot	PACF plot
Switzerland			
Sweden			
Germany			

Table: Training data sets and corresponding ACF,PACF plots.

Performance Evaluation

Table: Quantitative measures for different forecasting models on the Switzerland data

Model	1-Year ahead forecast			2-Year ahead forecast			3-Year ahead forecast		
	RMSE	MAE	MAPE	RMSE	MAE	MAPE	RMSE	MAE	MAPE
ARIMA	0.047	0.037	1.095	0.153	0.116	3.436	0.437	0.314	9.365
ANN	0.226	0.133	5.394	0.949	0.607	40.363	1.326	0.933	115.176
NNAR	0.073	0.048	1.715	0.209	0.140	4.775	0.498	0.340	10.924
Hybrid ARIMA+ANN	0.045	0.035	1.035	0.151	0.114	3.366	0.435	0.311	9.295
Hybrid ARIMA+SVM	0.048	0.038	1.117	0.154	0.117	3.459	0.438	0.315	9.387
Hybrid ARIMA+NNAR	**0.036**	**0.028**	**0.838**	**0.142**	**0.104**	**3.093**	**0.427**	**0.301**	**9.017**

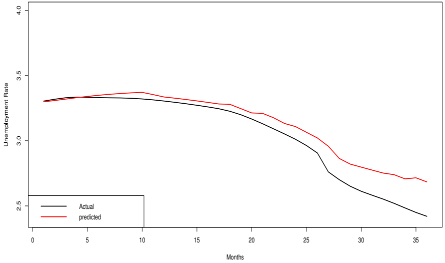


Fig: Actual vs predicted forecasts (using ARIMA+NNAR model) of Switzerland Data set

Merits & Discussions

- The hybridization approach studies the relationship between linear and nonlinear components of the econometric time series.
- The Additive method is appropriate for explaining variations of economic and business data where there are interactions between linear and nonlinear time series.
- The proposed hybrid model assume that the residuals from the linear model will contain only the nonlinear relationship. However, one may not always guarantee that the residuals of the linear component may comprise valid nonlinear patterns.
- This model also supposes that the linear and nonlinear patterns of a time series can be separately modeled by different models and then the forecasts can be combined together and this may degrade performance, if it is not true.

On Asymptotic Stationarity

ARIMA model has the in-built mechanism to transform a nonstationary time series into a stationary one and then it models the remainder by a stationary process. This is done by simple differencing to transform nonstationary ARIMA into stationary.

Consider the stochastic difference equation:

$$\varepsilon_t \quad = \quad f(\varepsilon_{t-1}, \varepsilon_{t-2}, ..., \varepsilon_{t-p}, \theta) + \varsigma_t, \tag{0.10}$$

where ς_t is an i.i.d. white noise and $f(., \theta)$ is a feedforward neural network with weight parameter θ. This is called an NNAR process of order p and has k hidden nodes in its one hidden layer. Thus, we refer the model as NNAR(p, k) model.

We consider the following architecture:

$$f(\underline{\varepsilon}) \quad = \quad c_0 + \sum_{i=1}^{k} w_i \sigma\left(a_i + b_i' \underline{\varepsilon}\right) \tag{0.11}$$

Let ε_t denote a time series generated by a nonlinear autoregressive process as defined in (0.10). Let $E(\varepsilon_t) = 0$, then f equals to the conditional expectation $E\left(\varepsilon_t | \varepsilon_{t-1}, ..., \varepsilon_{t-p}\right)$ is the best prediction for ε_t in the L_2-minimization sense.

On Geometric Ergodicity

We use the following notation:

$$z_{t-1} = \left(\varepsilon_{t-1}, ..., \varepsilon_{t-p}\right)' ; F(z_{t-1}) = \left(f(z_{t-1}), \varepsilon_{t-1}, ..., \varepsilon_{t-p+1}\right)' ; \hat{\varsigma}_t = \left(\varsigma_t, 0, ..., 0\right)'$$

Then we can write scalar AR(p) model in (0.10) as a first-order vector model,

$$z_t \quad = \quad F(z_{t-1}) + \hat{\varsigma}_t \ \text{ with } z_t, \hat{\varsigma}_t \in \mathbb{R}^p \tag{0.12}$$

Definition (Geometric ergodicity, Chan & Tong, 1985, AAP)

Let $\{z_t\}$, a markov chain, is said to be geometrically ergodic if there exists a probability measure $\Pi(A) = \lim_{t\to\infty} P(\varepsilon_t \in A)$ on the state space $(\mathbb{R}^p, \mathbb{B}, \mathbb{P})$, where $\mathbb{B}$ are Borel set on $\mathbb{R}^p$ and $\mathbb{P}$ be the Lebesgue measure, and for $\rho > 1$ and for all $z \in \mathbb{R}^p$,

$$\lim_{n\to\infty} \rho^n \| P\{z_{t+n} \in A | z_t = z\} - \Pi(A) \| \quad = \quad 0$$

where $\|.\|$ denotes the total variation and $P\{z_{t+n} \in A | z_t = z\}$ denote the probability of going from point z to set $A \in \mathbb{B}$ in n steps.

If the markov chain is geometrically ergodic then its distribution will converge to Π and the corresponding time series will be called asymptotically stationary (Chan & Tong, 1985, Advances in Applied Probability).

On Asymptotic Stationarity

It is also important to note that all neural network activation functions (like logistics or tan-hyperbolic) are continuous and compact functions with bounded range.

Lemma (Chakraborty et al. Computational Economics (2020))

Suppose $\{z_t\}$ is defined as in (0.10) and (0.12), F be a compact set can be decomposed as $F = F_m + F_n$, and the following conditions hold:
(i) $F_m(.)$ is continuous and homogeneous and $F_n(.)$ is bounded;
(ii) $E|\varsigma_t| < \infty$ and probability distribution function of ς_t is positive everywhere in $\mathbb{R}$;
then $\{z_t\}$ is geometrically ergodic.

Theorem (Chakraborty et al. Computational Economics (2020))

Let $E|\varsigma_t|^{1+\delta} < \infty$ for all $\delta > 1$ and the probability density function of ς_t is positive everywhere in $\mathbb{R}$ and $\{\varepsilon_t\}$ and $\{z_t\}$ are defined as in (0.10) and (0.12). Then if f is a nonlinear neural network as defined in (0.11), then $\{z_t\}$ is geometrically ergodic and $\{\varepsilon_t\}$ is asymptotically stationary.

- Theoretical results on asymptotic stationarity is important for predictions over larger intervals of time, for example, one might train the network on an available sample and then use the trained network to generate new data with similar properties than the training sample.
- The asymptotic stationarity guarantees that the model cannot have growing variance with time.

Simulation Study

A time series data have been synthesized in such a way that the mean between multiple segments in both the test and training data differ. The data consists of 165 points out of which 15 data points are kept as test samples (red-colored samples in the figure).

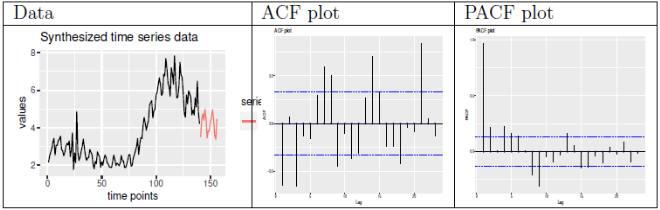


Table: Performance metrics with 15 points-ahead test set for synthesized data. Figures in ( ) indicate the values of the tuning parameters for each of the forecasting models.

Model	15-points ahead forecast			
	RMSE	MAE	MAPE	SMAPE
ARIMA(2,1,4)	0.718	0.609	1.689	1.607
ANN(10)	0.967	0.838	2.515	2.169
ARNN(16,8)	0.763	0.664	1.975	1.742
Hybrid ARIMA(2,1,4)-ARNN(8,4)	**0.597**	**0.465**	**1.322**	**1.245**

Conclusions

- In practice, it is often challenging to determine whether a time series under study is generated from a linear or nonlinear underlying process.
- In this chapter, we have built a novel hybrid model with a multiplicative approach that performs superior for forecasting unemployment rates.
- The proposed hybrid ARIMA+NNAR model filters out linearity using the ARIMA model and predicts nonlinear tendencies with the NNAR approach.
- In this work, we have also investigated the asymptotic behavior (stationarity and ergodicity) of the proposed hybrid approach using Markov chains and nonlinear time series analysis techniques.

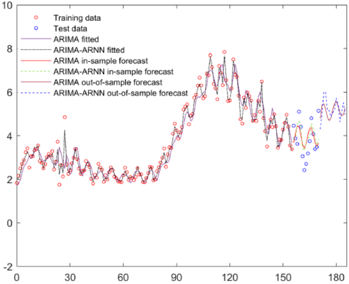


Figure: Plots of the proposed forecasting model for training, testing, and 15-points ahead forecast results on synthesized data.

Chapter 8: Conclusions and Future works

Conclusions & Future Work

- We developed some novel Hybrid Prediction models for various problems arising in classification and regressions.
- The problems arise from the area of Business Analytics, Quality Control, Macroeconomics, and Software Reliability.
- We considered the following prediction problems: Feature Selection cum Classification Problem, Imbalanced Classification Problem, Nonparametric Regression Problem, Bayesian + Frequentist approach, and Time Series Forecasting Problem.
- We studied several statistical properties of the proposed hybrid models.
- The scope of future research of the thesis will be to improve the proposed classifiers for imbalanced classification problem with concept shift in the data sets.
- Another scope of future research of the thesis will be to build Hybrid Models for Adversarial Machine Learning Problems.

Publications from the thesis

1. Tanujit Chakraborty, Swarup Chattopadhyay, and Ashis Kumar Chakraborty. "A novel hybridization of classification trees and artificial neural networks for selection of students in a business school", **Opsearch**. 55 (2018): 434-446. **(Read Online)**
2. Tanujit Chakraborty, Ashis Kumar Chakraborty, and C. A. Murthy. "A nonparametric ensemble binary classifier and its statistical properties", **Statistics & Probability Letters**. 149 (2019): 16-23. **(Read Online)**
3. Tanujit Chakraborty and Ashis Kumar Chakraborty. "Hellinger Net : A Hybrid Imbalance Learning Model to Improve Software Defect Prediction", **IEEE Transactions on Reliability**. **(Read Online)**
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