Department of Information and Computer Science

Advances in Extreme Learning Machines

Mark van Heeswijk

Aalto University

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Advances in Extreme Learning Machines

Mark van Heeswijk

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Aalto University
School of Science
Department of Information and Computer Science
Environmental and Industrial Machine Learning Group

Supervising professor
Aalto Distinguished Prof. Erkki Oja

Thesis advisor
Dr. Yoan Miche

Preliminary examiners
Prof. Guang-Bin Huang, Nanyang Technological University, Singapore
Prof. Jonathan Tapson, University of Western Sydney, Australia

Opponent
Prof. Donald C. Wunsch, Missouri University of Science & Technology, United States

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Abstract

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Abstract

Nowadays, due to advances in technology, data is generated at an incredible pace, resulting in large data sets of ever-increasing size and dimensionality. Therefore, it is important to have efficient computational methods and machine learning algorithms that can handle such large data sets, such that they may be analyzed in reasonable time. One particular approach that has gained popularity in recent years is the Extreme Learning Machine (ELM), which is the name given to neural networks that employ randomization in their hidden layer, and that can be trained efficiently. This dissertation introduces several machine learning methods based on Extreme Learning Machines (ELMs) aimed at dealing with the challenges that modern data sets pose. The contributions follow three main directions.

Firstly, ensemble approaches based on ELM are developed, which adapt to context and can scale to large data. Due to their stochastic nature, different ELMs tend to make different mistakes when modeling data. This independence of their errors makes them good candidates for combining them in an ensemble model, which averages out these errors and results in a more accurate model. Adaptivity to a changing environment is introduced by adapting the linear combination of the models based on accuracy of the individual models over time. Scalability is achieved by exploiting the modularity of the ensemble model, and evaluating the models in parallel on multiple processor cores and graphics processor units. Secondly, the dissertation develops variable selection approaches based on ELM and Delta Test, that result in more accurate and efficient models. Scalability of variable selection using Delta Test is again achieved by accelerating it on GPU. Furthermore, a new variable selection method based on ELM is introduced, and shown to be a competitive alternative to other variable selection methods. Besides explicit variable selection methods, also a new weight scheme based on binary/ternary weights is developed for ELM. This weight scheme is shown to perform implicit variable selection, and results in increased robustness and accuracy at no increase in computational cost. Finally, the dissertation develops training algorithms for ELM that allow for a flexible trade-off between accuracy and computational time. The Compressive ELM is introduced, which allows for training the ELM in a reduced feature space. By selecting the dimension of the feature space, the practitioner can trade off accuracy for speed as required.

Overall, the resulting collection of proposed methods provides an efficient, accurate and flexible framework for solving large-scale supervised learning problems. The proposed methods are not limited to the particular types of ELMs and contexts in which they have been tested, and can easily be incorporated in new contexts and models.

Keywords Extreme Learning Machine (ELM), high-performance computing, ensemble models, variable selection, random projection, machine learning

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Preface

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Espoo, March 2015,

Mark van Heeswijk

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List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.

I Mark van Heeswijk, Yoan Miche, Tiina Lindh-Knuutila, Peter A.J. Hilbers, Timo Honkela, Erkki Oja, and Amaury Lendasse. Adaptive Ensemble Models of Extreme Learning Machines for Time Series Prediction. In *LNCS 5769 - Artificial Neural Networks, ICANN'09: International Conference on Artificial Neural Networks*, pp. 305-314, September 2009.

II Mark van Heeswijk, Yoan Miche, Erkki Oja, and Amaury Lendasse. GPU-accelerated and parallelized ELM ensembles for large-scale regression. *Neurocomputing*, 74 (16): pp. 2430-2437, September 2011.

III Benoît Frenay, Mark van Heeswijk, Yoan Miche, Michel Verleysen, and Amaury Lendasse. Feature selection for nonlinear models with extreme learning machines. *Neurocomputing*, 102, pp. 111-124, February 2013.

IV Alberto Guillén, Maribel García Arenas, Mark van Heeswijk, Dušan Sovilj, Amaury Lendasse, Luis Herrera, Hector Pomares and Ignacio Rojas. Fast Feature Selection in a GPU Cluster Using the Delta Test. *Entropy*, 16 (2): pp. 854-869, 2014.

V Mark van Heeswijk, and Yoan Miche. Binary/Ternary Extreme Learning Machines. *Neurocomputing*, 149, pp. 187-197, February 2015.

VI Mark van Heeswijk, Amaury Lendasse, and Yoan Miche. Compressive ELM: Improved Models Through Exploiting Time-Accuracy Trade-offs. In *CCIS 459 - Engineering Applications of Neural Networks*, pp. 165-174, 2014.

Author's Contribution

Publication I: "Adaptive Ensemble Models of Extreme Learning Machines for Time Series Prediction"

This publication introduces an ensemble of ELMs for one-step-ahead time series prediction, with ensemble weights adapting after each prediction step, depending on the error of the individual models. This allows the ensemble to adapt to nonstationarities in the time series. Furthermore, various retraining strategies are explored for retraining the models on a sliding or growing window. The proposed method is tested on stationary and nonstationary time series. Experiments show that the adaptive ensemble model has low computational cost, and achieves a test error comparable to the best methods, while keeping adaptivity. The present author defined the problem together with the other authors, and was responsible for most of the coding, experiments, and writing of the article.

Publication II: "GPU-accelerated and parallelized ELM ensembles for large-scale regression"

This publication presents an ensemble of GPU-accelerated ELMs, which are trained in parallel on multiple GPUs, such that regression on large data sets can be performed in reasonable time. Furthermore, an efficient method based on PRESS statistics is exploited for model selection. The experiments show that competitive performance is obtained on the regression tasks, and that the GPU-accelerated and parallelized ELM ensemble achieves attractive speedups over using a single CPU. Finally, the proposed approach is not limited to a specific type of ELM and can be employed for a large variety of ELMs. The present author was responsible

for the proposal of the topic, coding, experiments, and most of the writing of the paper.

Publication III: "Feature selection for nonlinear models with extreme learning machines"

This publication explores a feature selection method based on Extreme Learning Machines, which returns a complete feature selection path representing the trade-off between the best feature subset for each subset size and the corresponding generalisation error. The present author contributed extensively to the definition of the problem and was responsible for the coding and write-up of the baseline experiments, consisting of various feature selection methods using the mutual information criterion.

Publication IV: "Fast Feature Selection in a GPU Cluster Using the Delta Test"

This publication proposes a 'genetic algorithm'-based feature selection method. The proposed algorithm is designed to be applied with very large datasets which could otherwise not be evaluated due to memory or time limitations. The workload is distributed over multiple nodes using the classical island approach. Furthermore, the main computational bottleneck (evaluation of the fitness function/Delta Test) is parallelized and evaluated across multiple GPUs. The present author was responsible for the initial implementation of the (multi-)GPU-accelerated Delta Test and writing the related parts of the paper.

Publication V: "Binary/Ternary Extreme Learning Machines"

This publication proposes two new ELM variants: Binary ELM, with a weight initialization scheme based on (0,1)-weights; and Ternary ELM, with a weight initialization scheme based on (-1,0,1)-weights. The motivation behind this approach is that these features will be from very different subspaces and therefore each neuron extracts more diverse information from the inputs than neurons with completely random features traditionally used in ELM. Experiments show that indeed ELMs with ternary weights generally achieve lower test error, and additionally are more ro-

bust to irrelevant and noisy variables. Since only the weight generation scheme is adapted, the computational time of the ELM is unaffected, and the improved accuracy, added robustness and the implicit variable selection of Binary ELM and Ternary ELM come for free. The present author was responsible for the proposal of the topic, coding, experiments, and most of the writing of the paper.

Publication VI: "Compressive ELM: Improved Models Through Exploiting Time-Accuracy Trade-offs"

This publication investigates the trade-off between the time spent optimizing and training several variants of the Extreme Learning Machine, and their final performance. Ideally, an optimization algorithm finds the model that has best test accuracy from the hypothesis space as fast as possible, and this model is efficient to evaluate at test time as well. However, in practice, there exists a trade-off between training time, testing time and testing accuracy, and the optimal trade-off depends on the user's requirements. The proposed model in this publication, the Compressive Extreme Learning Machine, allows for a time-accuracy trade-off by training the model in a reduced space. Experiments indicate that this trade-off is efficient in the sense that on average more time can be saved than accuracy lost and therefore might provide a mechanism for obtaining better models in less time. The present author was responsible for the proposal of the topic, coding, experiments, and most of the writing of the paper.

List of Abbreviations

AIC	Akaike Information Criterion
BIC	Bayesian Information Criterion
BIP	Batch Intrinsic Plasticity
BW	Backward
CV	Cross-Validation
DT	Delta Test
ELM	Extreme Learning Machine
FSP	Feature Selection Path
FW	Forward
FWBW	Forward-Backward
GPU	Graphics Processing Unit
LARS	Least Angle Regression
LOO	Leave One Out
MI	Mutual Information
MSE	Mean Square Error
MRSR	Multiresponse Sparse Regression
PRESS	Predictive Sum of Squares
RMSE	Root Mean Square Error
SLFN	Single-Layer Feedforward Network
SET	Sparsity Error Trade-off
SVD	Singular Value Decomposition
TR	Tikhonov-Regularized

List of Notations

$\mathbf{x}$, $\mathbf{y}$	vectors
$\mathbf{X}$, $\mathbf{Y}$	matrices
$\hat{y}$	estimation of y
$\mathbf{x}_i$	i^{th}sample
$\mathbf{x}_{ij}$	i^{th}sample, j^{th}entry
N	number of samples
d	dimension of input samples
M	number of hidden neurons
$\mathbf{w}_i$	hidden layer weights of neuron i
b_i	hidden layer bias of neuron i
$f(\cdot)$	(transfer) function
$\mathbf{H}$	hidden layer output matrix
$\mathbf{H}^{\dagger}$	Moore-Penrose pseudo-inverse of $\mathbf{H}$
$\boldsymbol{\beta}$	hidden layer output weights
$\lvert\cdot\rvert$	absolute value
$\lVert\cdot\rVert$	L2 norm
δ	Delta Test

1. Introduction

1.1 Motivation and scope

Due to technological advances, nowadays data gets generated at an ever-increasing pace and the size and dimensionality of data sets continue to grow by the day. Therefore, it is important to develop efficient and effective machine learning methods, that can be used to analyze this data and extract useful knowledge and insights from this wealth of information.

In recent years, Extreme Learning Machines (ELMs) have emerged as a popular framework in machine learning. ELMs are a type of feed-forward neural networks characterized by a random initialization of their hidden layer weights, combined with a fast training algorithm. The effectiveness of this random initialization and their fast training makes them very appealing for large data analysis.

Although in theory ELMs have been proven to be universal approximators and the random initialization of the hidden neurons should be sufficient to solve any approximation problem, in practice it matters greatly how many samples are available for training; whether there are any outliers in the data; and which variables are used as inputs. Therefore, proper care needs to be taken to obtain a robust and accurate model, and prevent overfitting. Furthermore, even though ELMs have efficient training algorithms, due to the size of modern data sets, ELMs can benefit from strategies for accelerating their training.

The focus of this thesis therefore is on developing efficient, and effective ELM-based methods that are specifically suited for handling the challenges posed by modern data sets. The contributions of the dissertation are along three directions, described in the following section.

1.2 Contributions of the thesis

Firstly, **ELM-based ensemble methods** are developed, which adapt to context and can scale to large data. The stochastic nature of ELMs makes them particularly suited for ensembling, since each ELM tends to make different errors when modeling data. By combining them in an ensemble model, these errors are averaged out, resulting in a more accurate model. In particular, Publication I introduces an adaptive ensemble of ELMs, which allows for adapting to nonstationarities in the data by adjusting the linear combination of the models based on their accuracy over time. Publication II on the other hand, is aimed at reducing the computational time of the ensemble model, such that it may scale to larger data. Scalability is achieved by exploiting the modularity of the ensemble model, and evaluating its constituent models in parallel on multiple processor cores and by accelerating their training by performing it on graphical processing units (GPUs). Furthermore, an efficient method (based on PRESS-statistics) is exploited for fast model selection.

Secondly, **variable selection approaches based on ELM and Delta Test** are developed for reducing the dimensionality of the data by selecting only the relevant variables. This, in turn, results in more accurate and efficient models. In particular, Publication III introduces a new variable selection method based on ELM, which is shown to be a competitive alternative to traditional variable selection methods. Publication IV focuses on variable selection with a genetic algorithm using the Delta Test criterion for estimating the accuracy a nonlinear model can achieve for a given variable subset. The scalability of variable selection using Delta Test is achieved by accelerating it on GPU, and by parallelizing the workload over multiple cluster nodes. Finally, besides these explicit variable selection methods, Publication V develops a new weight initialization scheme for ELM consisting of binary and ternary sparse weights. As a result, the hidden neurons extract more diverse information from the data, which results in more accurate and effective models. This weight scheme is shown to perform implicit variable selection. Since only the weight scheme is adapted, the resulting increased robustness and accuracy come for free and at no increase in computational cost.

Finally, training algorithms for ELM are developed that allow for a **flexible trade-off between accuracy and computational time**. In particular, Publication VI introduces the Compressive ELM, which provides a

way to reduce the computational time by performing the training of ELM in a reduced feature space. This allows for a flexible time-accuracy trade-off (and might provide a way to obtain more accurate models in less time).

Overall, the resulting collection of proposed methods provides an efficient, accurate and flexible framework for solving large-scale supervised learning problems. The developed methods are not limited to the particular types of ELMs and contexts in which they have been tested, and may readily be adapted to new contexts and models.

1.3 Structure of the thesis

The remainder of this thesis gives an introduction to topics and theory relevant to the thesis, and highlights results from the included publications. In particular, chapter 2 discusses the general machine learning background relevant to the thesis. Chapter 3 introduces Extreme Learning Machines and some of its variants. Chapter 4 discusses ensemble models and contributions to ensembles of ELMs. Chapter 5 gives an overview of feature selection and related contributions. Chapter 6 discusses the compressive ELM and finally, Chapter 7 provides conclusions and future work.

2. Machine learning

"All models are wrong, but some are useful."

– George Box

Machine learning is a challenging field, which is concerned with the problem of building models that can extract useful information or insights from given data. As mentioned in the introduction already, the size and dimensionality of the data sets become larger by the day, and it is therefore important to develop efficient computational methods and algorithms that are able to handle these large data sets, such that the machine learning tasks can still be performed in reasonable time.

This chapter gives an overview of the basic concepts of machine learning relevant to this thesis, and on supervised learning in particular.

2.1 Unsupervised learning

In machine learning, at least two different types of learning can be distinguished: supervised learning and unsupervised learning (Bishop, 2006; Murphy, 2012; Alpaydin, 2010). In unsupervised learning, no target variables are given, and the task is to extract useful patterns or information from just $(\mathbf{x_i})_{i=1}^{N}$, where $\mathbf{x}_i$ refers to the i^{th} sample in a data set of N samples (e.g. corresponding to images). Examples of unsupervised learning include clustering and principal component analysis (PCA), where the algorithm tries to discover latent structure in the data. Other uses of unsupervised learning are visualization or exploration of the data.

2.2 Supervised learning

In supervised learning on the other hand, the goal is to model the relationship between a set of explanatory variables $\mathbf{x_i}$ and the corresponding target variable (or target variables) y_i, where subscript i indicates the sample. That is, given a set of data $(\mathbf{x_i}, y_i)_{i=1}^{N}$, model the relationship between inputs $\mathbf{x_i}$ and outputs y_i as a function f, such that $f(\mathbf{x_i})$ matches y_i as closely as possible. This is often referred to as functional approximation.

In case the target variable $y_i \in \mathbb{R}$, this is known as regression. In case y_i corresponds to a category or class, this is known as classification.

2.2.1 Functional approximation

An example of a functional approximation problem is time series prediction, where the task is to predict future values of a particular time series based on its past values. One possibility for using past data to predict the future would be to model the next value of the time series (at time $t + 1$) as a function of the values in the previous d time steps. Having recast the task of time series prediction as a functional approximation (or regression) problem, the problem of one-step ahead time series prediction can be described as follows

$$\hat{y}_i = f(\mathbf{x}_i, \boldsymbol{\beta}) \tag{2.1}$$

where $\mathbf{x}_i$ is a $1 \times d$ vector $[x(t - d + 1), \ldots, x(t)]$ with d the number of past values that are used as input, and $\hat{y}_i$ the approximation of $x(t + 1)$. Note the difference between $\mathbf{x}_i$ and $x(t)$.

Depending on what kind of relation is expected to exist between the input variables and output variables of a given problem, the regression is performed on either the input variables themselves or nonlinear transformations of them, e.g. like in neural networks which perform linear regression on nonlinear transformations of the input variables (i.e. the outputs of the hidden layer) and the target variables.

2.2.1.1 Linear regression

In linear regression, as the name suggests, the function f becomes a linear combination of the input variables, i.e.

$$f(\mathbf{x}_i, \boldsymbol{\beta}) = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_d x_{id}. \tag{2.2}$$

Given a number of training samples $(\mathbf{x}_i, y_i)_{i=1}^N$, the inputs $\mathbf{x_i}$ and targets y_i can be gathered in matrices, such that the linear system can be written as

$$\mathbf{X}\boldsymbol{\beta} = \mathbf{Y} \tag{2.3}$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & x_{N2} & \cdots & x_{Nd} \end{bmatrix}, \quad \mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \tag{2.4}$$

d is the number of inputs and N the number of training samples. The matrix $\mathbf{X}$ is also know as the regressor matrix and each row contains an input and a column of ones corresponding to β_0, while the corresponding row in $\mathbf{Y}$ contains the target to approximate.

The weight vector $\boldsymbol{\beta}$ which results in the least mean square error (MSE) approximation of the training targets $\mathbf{Y}$ given input $\mathbf{X}$ can now be computed as follows (Bishop, 2006):

$$\begin{aligned} \mathbf{X}\boldsymbol{\beta} &= \mathbf{Y} \\ \mathbf{X}^T\mathbf{X}\boldsymbol{\beta} &= \mathbf{X}^T\mathbf{Y} \\ (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X})\boldsymbol{\beta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\ \boldsymbol{\beta} &= (\mathbf{X^T X})^{-\mathbf{1}}\mathbf{X^T} = \mathbf{X}^\dagger\mathbf{Y} \end{aligned}$$

where $\mathbf{X}^\dagger$ is known as the pseudo-inverse or Moore-Penrose inverse (Rao and Mitra, 1971).[1]

Furthermore, since the approximation of the output for given $\mathbf{X}$ and $\boldsymbol{\beta}$ is defined as $\hat{\mathbf{Y}} = \mathbf{X}\boldsymbol{\beta}$

$$\begin{aligned} \hat{\mathbf{Y}} &= \mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\ &= \mathrm{HAT} \cdot \mathbf{Y} \end{aligned}$$

where the HAT-matrix is the matrix that transforms the output $\mathbf{Y}$ into the approximated output $\hat{\mathbf{Y}}$. It is defined as $\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ and plays an important role in this thesis, as it provides an efficient way to estimate the

[1] The matrix $\mathbf{X}^T\mathbf{X}$ is invertible (non-singular) exactly when its rank equals dimension d, which is usually the case if $N \geq d$. In case $N < d$, $\mathbf{X}^\dagger = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T)^{-1}$

expected performance of a linear model, and therefore an efficient way to perform model selection.

2.2.1.2 Linear basis function models

Instead of doing regression on the input variables, one can also perform regression on non-linear transformations of the input variables. These nonlinear transformations are often referred to as *basis functions*, and the approach as a whole as *basis function* expansion. This approach is more powerful than linear regression and can, given enough basis functions, approximate any given function under the condition that these basis functions are infinitely differentiable. In other words, they are universal approximators (Hornik et al., 1989; Cybenko, 1989; Funahashi, 1989).

2.2.2 Model structure selection

In supervised learning, a model tries to learn the relationship between a set of inputs and a set of outputs. This could for example be a set of images that needs to be classified into a number of categories, or a time series prediction problem, in which future values of that time series need to be predicted given its past values and possibly other external information.

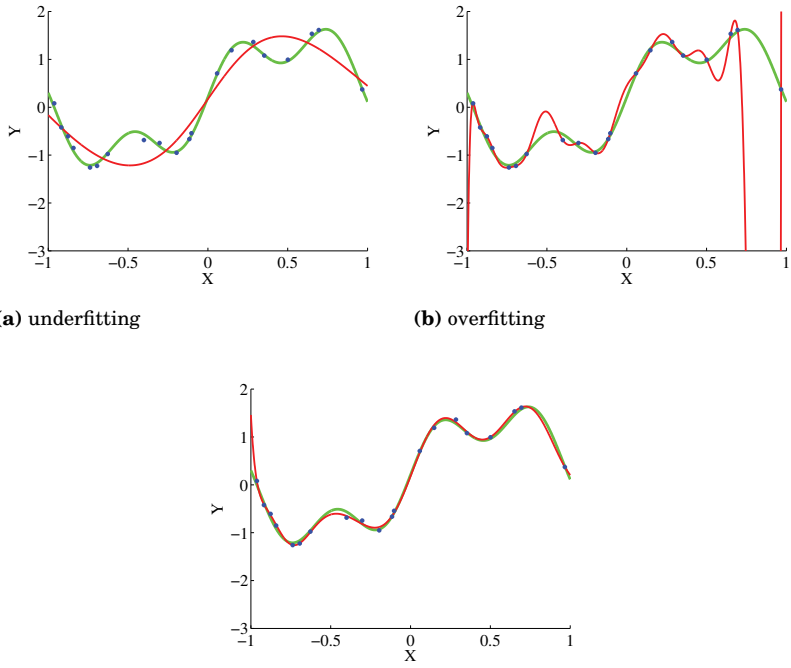
The model that is used to represent and learn this relationship has a certain structure determined by its parameters and a corresponding learning algorithm with its hyper-parameters. The class of possible models is sometimes known as the hypothesis space (Alpaydin, 2010), and it is up to the learning algorithm to find the best model from the hypothesis space (in terms of some criterion like e.g. accuracy) that models the relationship between input and output data best, and can consequently be used to accurately predict the output for future unseen inputs.

In optimizing the structure of a model, many models with different structure and parameters are evaluated according to some criteria. For example, in case of neural networks the models could differ in terms of the number or type of neurons in the hidden layer; how many and which variables are taken as input; and the algorithm and parameters used to train the neural network.

A commonly used criterion is the accuracy of the model. However, since the future samples are not necessarily the same as the currently available samples (e.g. due to noise or other changes in the environment), it is important that the model generalizes to this new unseen data: i.e. it is not enough to perfectly model the training data.

2.2.2.1 *Motivation*

In selecting the right model structure, one of the aspects often optimized is the model complexity (e.g. the number of hidden neurons in a neural network). If the model is too complex, it will perfectly fit the training data, but will have bad generalization on data other than the training data. On the other hand, if the model is too simple, it will not be able to approximate the training data at all. These cases are known as overfitting and underfitting, respectively, and are illustrated in Figure 2.1. If the model is too simple, it is not able to learn the functional mapping between the inputs and the outputs; if the model is too complex on the other hand, it perfectly approximates the points it was trained on, but exhibits poor generalization performance and does not approximate the underlying function of the data very well.



(a) underfitting

(b) overfitting

(c) good fit

Figure 2.1. Output of various models (*red line*), trained on a number of points (*blue dots*) of the underlying function (*green line*) (van Heeswijk, 2009)

From these examples, it becomes clear that there is a trade-off between accuracy of the model on the training set, and the generalization performance of the model on the test set. Furthermore, there is an optimal complexity of the model, for which the trained model generalizes well to

the unseen test set.

In order to determine the optimal complexity, the expected generalization error needs to be estimated, and it needs to be determined without using the test set. Here, three approaches are discussed: validation, k-fold cross-validation and leave-one-out cross-validation. See (Bishop, 2006) and (Efron and Tibshirani, 1993) for more detailed information on model (structure) selection methods.

2.2.3 Model selection methods

A good model performs well on the training set, and the input-output mapping that the model learned from the training set transfers well to the test set. In other words, the model approximates the underlying function of the data well and has good generalization.

How well a model generalizes can be measured in the form of the *generalization error*. In case of a functional approximation problem, and using an ℓ_2 loss function, the generalization error can be defined as

$$E_{gen}(\boldsymbol{\theta}) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i, \boldsymbol{\theta}))^2 \tag{2.5}$$

where N is the number of samples, $\mathbf{x}_i$ is the d-dimensional input, $\boldsymbol{\theta}$ contains the model parameters, and y_i is the output corresponding to input vector $\mathbf{x}_i$.

Of course, in reality there is no infinite number of samples, but only a limited amount of samples in the form of a *training set* and a *test set*, consisting of samples that the model will be trained on and samples that the model will be tested on, respectively. Therefore, the training set is to be used to estimate the generalization performance, and thus the quality, of a given model.

Below, three different methods are discussed that are often used in model selection and the estimation of the generalization error of a model.

Validation In validation, part of the training set is set aside in order to evaluate the generalization performance of the trained model. If the indices of the samples in the validation set are denoted by val and the indices of the samples in the full training set by $train$, then the estimation of the generalization error is defined as

$$\hat{E}_{gen}^{\mathrm{VAL}}(\boldsymbol{\theta}^*) = \frac{1}{|val|} \sum_{i\in val} (y_i - f(\mathbf{x}_i, \boldsymbol{\theta}^*_{train\setminus val}))^2 \tag{2.6}$$

where $\boldsymbol{\theta}^*_{train \setminus val}$ denotes the model parameters trained on all samples that are in the training set, but not in the validation set. Note that once the validation procedure and model selection is completed, the model is trained on the full training set.

The problem with this validation procedure is that it is not very reliable, since a small part of the data is held out for validation, and it is unknown how representative this sample is for the test set.

k-Fold cross-validation k-fold cross-validation is similar to validation, except that the training set is divided into k parts (typically $k = 10$), each of which is used as validation set once, while the rest of the samples are used for training. The final estimation of the generalization error is the mean of the generalization errors obtained in each of the k folds

$$\hat{E}^{kCV}_{gen}(\boldsymbol{\theta}^*) = \frac{1}{k}\sum_{s=1}^{k}\left[\frac{1}{|val_s|}\sum_{i \in val_s}(y_i - f(\mathbf{x}_i, \boldsymbol{\theta}^*_{train \setminus val_s}))^2\right] \tag{2.7}$$

where $\boldsymbol{\theta}^*_{train \setminus val_s}$ denotes the model parameters trained on all samples that are in the training set, but not in validation set val_s.

Although k-fold cross-validation gives a better estimation of the generalization error, it is computationally more intensive than validation, since the validation is performed k times.

Leave-one-out cross-validation Finally, Leave-one-out (LOO) cross-validation is a special case of k-fold cross-validation, namely the case where $k = N$. The models are trained on N training sets, each of which omits exactly one of the samples. The left-out sample is used for validation, and the final estimation of the generalization error is the mean of the N obtained errors

$$\hat{E}^{LOO}_{gen}(\boldsymbol{\theta}^*) = \frac{1}{N}\sum_{i=1}^{N}(f(\mathbf{x}_i, \boldsymbol{\theta}^*_{-i}) - y_i)^2 \tag{2.8}$$

where $\boldsymbol{\theta}^*_{-i}$ denotes the model parameters trained on all samples that are in the training set except on sample i.

Due to the fact that better use is made of the training set, the LOO cross-validation gives the more reliable estimate of the generalization error. Although the amount of computation for LOO cross-validation might seem excessive, for linear models, a closed-form formula exists that can compute all leave-one-out errors efficiently.

Leave-one-out computation using PRESS statistics Although it might seem like a lot of work to compute the leave-one-out errors (i.e. N models would

need to be trained), the leave-one-out errors of a linear model can be computed efficiently from its residuals (i.e. the errors of the trained model on the training set) through PRESS (Prediction Sum of Squares) statistics (Allen, 1974; Myers, 1990)

$$\text{PRESS} = \sum_{i=1}^{N}(y_i - \mathbf{x}_i\boldsymbol{\beta}_{-i})^2 = \sum_{i=1}^{N}(y_i - \hat{y}_{i,-i})^2 = \sum_{i=1}^{N}(\epsilon_{i,-i})^2.$$

where $\epsilon_{i,-i}$ denotes the leave-one-out error when sample i is left out (also known as the PRESS residual); y_i denotes the target output specified by sample i from the training set, and $\boldsymbol{\beta}_{-i}$ denotes the weight vector obtained when training the linear model on the training set with sample i left out.

The PRESS residuals $\epsilon_{i,-i}$ can be computed efficiently as follows

$$\begin{aligned}
\epsilon_{i,-i} &= \frac{\epsilon_i}{1 - \mathbf{x}_{i\cdot}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_{i\cdot}^T} \\
&= \frac{y_i - \hat{y}_i}{1 - \mathbf{x}_{i\cdot}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_{i\cdot}^T} \\
&= \frac{y_i - \mathbf{x}_i\boldsymbol{\beta}}{1 - \mathbf{x}_{i\cdot}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_{i\cdot}^T} \\
&= \frac{y_i - \mathbf{x}_i\boldsymbol{\beta}}{1 - h_{ii}}
\end{aligned} \tag{2.9}$$

where $\mathbf{x}_{i\cdot}$ is the i^{th} row of matrix $\mathbf{X}$, h_{ii} is the i^{th} element on the diagonal of the HAT matrix $\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$, which was already encountered in Section 2.2.1.1. Therefore, the model only needs to be trained once on the entire training set in order to obtain $\boldsymbol{\beta}$, as well as the HAT matrix. Once the model is trained, all the PRESS residuals can easily be derived using Equation 2.9. Obviously, this involves a lot less computation than training the model for all N possible training sets.

Although PRESS statistics define an efficient way to compute the leave-one-out errors for linear models, this approach is not limited to models that are linear in the input variables: e.g. it can also be used in models that are linear in nonlinear transformations of the input variables, an important class of which is Extreme Learning Machines.

3. Extreme Learning Machines

"Not all those who wander are lost."

– J.R.R. Tolkien, *Lord of the Rings*

Extreme Learning Machines (ELMs) (Huang et al., 2004, 2006b) is the name for a collection of neural network models, which employ randomization of the hidden layer weights and a fast training algorithm. Typically, instead of optimizing the hidden layer and output weights through an iterative algorithm like backpropagation (Rumelhart et al., 1986), ELMs initialize the hidden layer randomly and training consists of solving the linear system defined by the hidden layer outputs and the targets. Despite the hidden layer weights being random, it has been proven that the ELM is still capable of universal approximation of any non-constant piecewise continuous function (Huang et al., 2006a; Huang and Chen, 2007, 2008). Due to its speed and broad applicability, the ELM framework has become very popular in the past decade.

The goal of this chapter is not to give an exhaustive overview of the entire ELM literature, nor is the goal to include every single proposed ELM variant. Rather, the goal is to give a birds-eye view of Extreme Learning Machines; to put them in historical context; and to identify some of the learning principles used. For example, an ELM variant might include L1 regularization, L2 regularization, or might be pre-trained in some way. The amount of possible combinations of these learning principles (and thus the number of ELM variants) increases rapidly, yet the number of possible ways to optimize an ELM is relatively limited. The focus in this chapter will be mainly on variants related to the models developed in this thesis. For a more complete overview of ELM variants and applications, the reader is referred to Huang et al. (2011, 2015).

3.1 Historical context

The idea of randomization of the hidden layer of neural networks has become very popular under the name Extreme Learning Machines and the name has become associated with a vast assortment of different models and variants of neural networks with randomized weights, including Single-Layer Feedforward Networks (SLFNs) (Huang et al., 2006b), kernelized SLFNs (Frénay and Verleysen, 2010, 2011; Huang et al., 2010), and deep architectures (Kasun et al., 2013).

The idea of randomization of the hidden layer in neural networks has been proposed several times. For example, the Random Vector Functional Link (RVFL) network (Pao and Takefuji, 1992; Pao et al., 1994; Igelnik and Pao, 1995) incorporates random hidden layer weights and biases, and direct connections between the input layer and output layer. Furthermore, several authors (Schmidt et al., 1992; te Braake and van Straten, 1995; te Braake et al., 1996; Chen, 1996; te Braake et al., 1997) introduced neural networks with a randomly initialized hidden layer, trained using the pseudo-inverse. This approach has also been used in the past for initializing the weights of a neural network (Yam and Chow, 1995; Yam et al., 1997; Yam and Chow, 2000) before training it with e.g. backpropagation. Finally, more recently, (Widrow et al., 2013) proposed the No-Prop algorithm, which has a random hidden layer and uses the LMS algorithm for training the output weights, rather than the pseudo-inverse. For an overview of how ELM compares to other methods incorporating randomization, see (Wang and Wan, 2008; Huang, 2008, 2014).

Although the idea of randomization in neural networks appears elsewhere, it cannot be denied that with the development of the Extreme Learning Machine over the past decade, the idea and theory of using randomization in neural networks has really come to fruition, and has been developed into a framework (rather than a single method) covering many machine learning methods, the uniting factor being the fact that some sort of random basis expansion / randomized hidden layer is used. Along with these methods, many theoretical and empirical results have been developed regarding the effectiveness of randomized features (Huang et al., 2015).

3.2 Standard ELM algorithm

The basic ELM algorithm for training Single-Layer Feedforward Neural Networks (SLFN) was first described in (Huang et al., 2006b). As mentioned, the key idea of ELM is the random initialization of the hidden layer weights and the subsequent training consists of computing the least-squares solution to the linear system defined by the hidden layer outputs and targets. An overview of the structure of an ELM is given in Figure 3.1 and the algorithm for training this network, as described in (Huang et al., 2006b), can be summarized as follows.

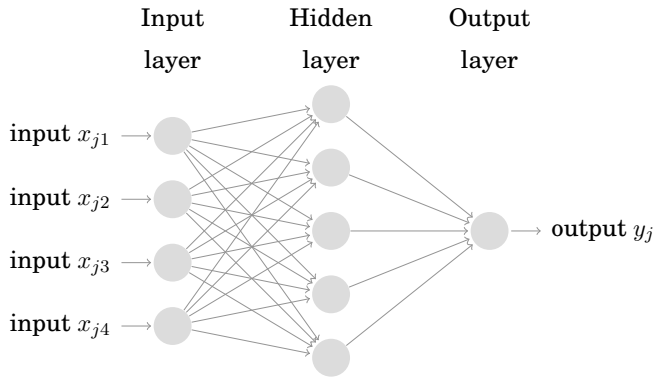


Figure 3.1. A schematic overview of an ELM

Consider a set of N distinct samples $(\mathbf{x}_i, y_i)$ with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. Then, the output of an SLFN with M hidden neurons can be written as

$$\hat{y_j} = \sum_{i=1}^{M} \beta_i f(\mathbf{w}_i \mathbf{x}_j + b_i), j \in [1, N], \tag{3.1}$$

where $\hat{y}_j$ is its approximation to y_j, f is the activation function, $\mathbf{w}_i$ the input weight vector, b_i the hidden layer bias and β_i the output weight corresponding to the i^{th} neuron in the hidden layer.

In case the SLFN would perfectly approximate the data (meaning the error between the output $\hat{y_j}$ and the actual value y_j is zero), the relation would be

$$\sum_{i=1}^{M} \boldsymbol{\beta}_i f(\mathbf{w}_i \mathbf{x}_j + b_i) = y_j, j \in [1, N], \tag{3.2}$$

which can be written compactly as

$$\mathbf{H}\boldsymbol{\beta} = \mathbf{Y}, \tag{3.3}$$

where $\mathbf{H}$ is the hidden layer output matrix defined as

$$\mathbf{H} = \begin{pmatrix} f(\mathbf{w}_1\mathbf{x}_1 + b_1) & \cdots & f(\mathbf{w}_M\mathbf{x}_1 + b_M) \\ \vdots & \ddots & \vdots \\ f(\mathbf{w}_1\mathbf{x}_N + b_1) & \cdots & f(\mathbf{w}_M\mathbf{x}_N + b_M) \end{pmatrix} \tag{3.4}$$

and $\boldsymbol{\beta} = (\beta_1 \dots \beta_M)^T$ and $\mathbf{Y} = (y_1 \dots y_N)^T$. See Algorithm 1 for a summary of the ELM algorithm.

Algorithm 1 Standard ELM

Given a training set $(\mathbf{x}_i, y_i), \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$, a probability distribution from which to draw random weights, an activation function $f : \mathbb{R} \mapsto \mathbb{R}$ and M the number of hidden nodes:

1: - Randomly assign input weights $\mathbf{w}_i$ and biases b_i, $i \in [1, M]$;
2: - Calculate the hidden layer output matrix $\mathbf{H}$;
3: - Calculate output weights matrix $\boldsymbol{\beta} = \mathbf{H}^{\dagger}\mathbf{Y}$.

The proposed solution to the equation $\mathbf{H}\boldsymbol{\beta} = \mathbf{Y}$ in the ELM algorithm, as $\boldsymbol{\beta} = \mathbf{H}^{\dagger}\mathbf{Y}$ has three main properties making it an appealing solution:

1. It is one of the least-squares solutions to the mentioned equation, hence the minimum training error can be reached with this solution;

2. It is the solution with the smallest norm among the least-squares solutions;

3. The smallest norm solution among the least-squares solutions is unique and is $\boldsymbol{\beta} = \mathbf{H}^{\dagger}\mathbf{Y}$.

3.3 Theoretical foundations

The strength of the Extreme Learning Machine is the fact that there is no need to iteratively tune of the randomly initialized network weights, which makes it very fast. Yet, despite the hidden neurons not being tuned, still an accurate network can be obtained.

Interpolation theory In particular, with the notations from Section 3.2, the Theorem presented in (Huang et al., 2006b) states that with randomly initialized input weights and biases for the SLFN, and under the condition that the activation function f is infinitely differentiable, then the hidden layer output matrix can be determined and will provide an approximation of the target values as good as wished (non-zero). Hence, the ELM can interpolate any set of samples as good as wished.

Theorem 1. *(Huang et al., 2006b). Given any small positive value $\epsilon > 0$, any activation function which is infinitely differentiable in any interval, and N arbitrary distinct samples $(\mathbf{x_i}, \mathbf{y_i}) \in \mathbb{R}^d \times \mathbb{R}^m$, there exists $M < N$ such that for any $\{\mathbf{w}_i, \mathbf{b}_i\}_{i=1}^{M}$ randomly generated from any interval of $\mathbb{R}^d \times \mathbb{R}$, according to any continuous probability distribution, with probability one, $\|\mathbf{H}\beta - \mathbf{T}\| < \epsilon$. Furthermore, if $M = N$, then with probability one, $\|\mathbf{H}\beta - \mathbf{T}\| = 0$.*

Universal approximation capability Besides being able to interpolate a finite set of samples, the ELM can also approximate any continuous target function f as good as wished.

Theorem 2. *(Huang et al., 2006a; Huang and Chen, 2007, 2008). Given any nonconstant piecewise continuous function $G : \mathbb{R}^d \to \mathbb{R}$, if span $\left\{G(\mathbf{a}, b, \mathbf{x}) : (\mathbf{a}, b) \in \mathbb{R}^d \mathbf{x} \mathbb{R}\right\}$ is dense in $L^2(\mathbb{R}^d)$ (i.e. the space of functions f on $\mathbb{R}^d$ which is a compact subset in the Euclidean space $\mathbb{R}^d$ such that $\int_{\mathbb{R}^d} |f(\mathbf{x})|^2 d\mathbf{x} < \infty$), then for any continuous target function f and any function sequence $\{G(\mathbf{w}_i, b_i, \mathbf{x})\}_{i=1}^{M}$ randomly generated according to any continuous sampling distribution, $\lim_{M\to\infty} \|f - f_M\| = 0$ holds with probability one if the output weights β_i are determined by ordinary least square to minimize $\left\|f(\mathbf{x}) - \sum_{i=1}^{M} \beta_i G(\mathbf{w}_i, b_i, \mathbf{x})\right\|$.*

3.4 Building a sound and robust architecture

Although the details of how an ELM is generated and trained differ between ELM schemes, most of these schemes can in some way be considered a variant of the following Algorithm 2, with the exact details of each step varying between schemes. The goal of each of these schemes is optimization of the hidden layer, such that as good as possible performance is achieved in the context in which the ELM is applied.

Algorithm 2 General structure of ELM schemes
Generate the ELM

- while not ready:
  - Generate candidate neurons
  - Select those candidate neurons that give the best value of some criterion

Train the ELM

- determine optimal output weights training targets and outputs of the hidden neurons from the generation step, using an optimization criteria like least squares or a regularized version of it.

Three main approaches for optimizing the ELM structure can be identified: constructive approaches; pruning approaches; and regularization approaches, as well as combinations of them.

The next subsections give an overview of these main approaches for building a sound and robust architecture, as well as a method for pretraining the ELM in order to optimize the amount of information the hidden layer neurons extract.

3.4.1 Incremental approaches

The incremental approach starts from a small network, and incrementally grows the hidden layer by adding new neurons until a certain stopping criterion is reached.

For example, the *Incremental ELM (I-ELM)* (Huang et al., 2006a) adds neurons which reduce the residual error of the model so far obtained as much as possible. While doing so, it only needs to train the weight for the neuron added in the current step. The final network is the one which achieves a certain target training error, or if it does not achieve that error before reaching a specified network size, the network of that specified size.

The *Convex Incremental ELM (CI-ELM)* (Huang and Chen, 2007) improves on the convergence speed of the I-ELM towards low-error models through the use of a convex optimization method, and correcting (but not

recomputing) the output weights with each incremental step.

As a final example, in the *Error-Minimized ELM (EM-ELM)* (Feng et al., 2009), more than one neuron can be added at the same time to grow the hidden layer. Additionally, the method has closed-form update rules for the weights when adding the new neurons, making the growing step fast.

3.4.2 Pruning approaches

Contrary to incremental approaches, pruning approaches first generate a larger than needed set of neurons. Given this set of candidate neurons, what remains is picking the best subset of M neurons for use in the SLFN.

In the Pruned ELM (Rong et al., 2008), a large set of candidate neurons is generated and ranked according to statistical relevance, using the χ^2 criterion or the information-gain criterion. An optimal threshold for this criterion is then determined using a separate validation set and the Akaike Information Criterion (AIC) (Akaike, 1974), after which the network is retrained on the entire training set.

The *Optimally Pruned ELM (OP-ELM)* (Miche et al., 2010) on the other hand, exploits the fact that the ELM is linear in the output of the hidden layer. This permits a fast and optimal ranking (in terms of training error) of the candidate neurons, using Least Angle Regression (LARS) (Efron et al., 2003), or Multiresponse Sparse Regression (MRSR) (Similä and Tikka, 2005). Once ranked, the optimal prefix of the sorted list of neurons is determined using the leave-one-out error, which can be efficiently computed using PRESS statistics (Allen, 1974; Myers, 1990).

Although the term 'pruned' suggest that the network architecture is being built starting from the largest network, and neurons are removed one-by-one, in fact the above approaches are quite similar to the incremental approach. The difference is that instead of randomly generating new neurons at each step, the entire candidate list of neurons is generated and ranked as a first step in the algorithm, and the neurons to be added are taken from that ranked candidate list of neurons. Therefore, the difference between the incremental and pruning approach is not that clear-cut.

For example, a recently proposed variant of the OP-ELM (which adds a number of regressors in each step of an MRSR-like algorithm, rather than a single one) was called the *Constructive Multi-output ELM* (Wang et al., 2014).

3.4.3 Regularization approaches

As an alternative to selecting the subset of hidden neurons, it is also possible to generate a large enough set of hidden neurons, and prevent overfitting by properly regularizing the network.

The *Regularized ELM (R-ELM)* (Deng et al., 2009) for example, is an approach in which the set of candidate neurons is fixed and taken large enough, while L2 regularization is used to prevent overfitting.

Finally, the *Tikhonov Regularized OP-ELM (TROP-ELM)* (Miche et al., 2011) is a variant of the OP-ELM, which efficiently incorporates the optimization of an L2 regularization parameter in the OP-ELM by integrating it in the SVD approach to computing pseudo-inverse $\mathbf{H}^{\dagger}$. This way, besides the advantage of sparsity, the output weights remain small and overfitting is prevented.

3.4.4 ELM pre-training

As it is extensively used in Publication V and Publication VI, in this section reviews intrinsic plasticity, as well as its adaptation to ELM (BIP-ELM) by (Neumann and Steil, 2011, 2013).

3.4.4.1 Motivation

Although ELMs are universal approximators, since often there are only limited training samples available. Therefore, it is important that the hidden layer neurons extract as much information as possible from the inputs.

A recently proposed pre-training method that achieves this is Batch Intrinsic Plasticity (BIP) (Neumann and Steil, 2011, 2013), which makes the ELM more robust by adapting the randomly generated hidden layer weights and biases such that each neuron achieves an exponential output distribution with a specified mean, and the amount of information that the hidden layer extracts from the limited amount of training samples is optimized.

Furthermore, the mechanism of intrinsic plasticity is one that is orthogonal to all the above-mentioned approaches. Namely, it generally takes place right after generating the random weights of the neurons, and its result is subsequently used in the further optimization, pruning and training of the ELM. As such, it can be used in combination with most other ELM approaches.

3.4.4.2 Intrinsic Plasticity

The concept of intrinsic plasticity has a biological background and refers to the fact that neurons adapt in such a way that they maximize their entropy (and thus the amount of information transmitted), while keeping the mean firing rate low. Intrinsic plasticity has been first used in papers regarding reservoir computing, recurrent neural networks, liquid state machines and echo state networks as a learning rule which maximizes information transmitted by the neurons (Triesch, 2005a,b; Verstraeten et al., 2007).

The information transmission of neurons is maximized by having the neuron outputs approximate an exponential distribution, which is the maximum entropy distribution among all positive distributions with fixed mean (Steil, 2007).

Furthermore, as (Verstraeten et al., 2007) notes in the context of reservoir computing, reservoirs are constructed in a stochastic manner, and the search for a method to construct a priori suitable reservoirs that are guaranteed or likely to offer a certain performance is an important line of research. Intrinsic plasticity is such a method which aims at constructing a network which is likely to give good performance. The recent study (Neumann et al., 2012) provides an in-depth analysis of intrinsic plasticity pre-training, and shows that it indeed results in well-performing networks with an impressive robustness against other network parameters like network size and strength of the regularization.

3.4.4.3 (Batch) Intrinsic Plasticity: BIP-ELM

In (Neumann and Steil, 2011, 2013; Neumann, 2013) the principle of intrinsic plasticity is transferred to ELMs and introduced as an efficient pre-training method, aimed at adapting the hidden layer weights and biases, such that the output distribution of the hidden layer is shaped like an exponential distribution. The motivation for this is that the exponential distribution is the maximum-entropy distribution over all distributions with fixed mean, maximizing the information transmission through the hidden layer. The only parameter of batch intrinsic plasticity is the mean of exponential distribution. This parameter determines the exact shape of the exponential distribution from which targets will be drawn, and can be set in various ways, as explained below.

Following (Neumann and Steil, 2011), the algorithm can be summarized as described as below.

Given the inputs $(\mathbf{x}_1, \ldots, \mathbf{x}_N) \in \mathbb{R}^{N \times d}$ and input matrix $\mathbf{W}^{in} \in \mathbb{R}^{d \times M}$ (with N the number of samples in the training set, d the dimensionality of the data, and M the number of neurons), the synaptic input to neuron i is given by $s_i(k) = \mathbf{x}_k \mathbf{W}^{in}_{\cdot i}$. Now, it is possible to adapt slope a_i and bias b_i, such that the desired output distribution is achieved for neuron output $h_i = f(a_i s_i(k) + b_i)$. To this end, for each neuron random targets $\mathbf{t} = (t_1, t_2, \ldots, t_N)$ are drawn from the exponential distribution with a particular mean, and sorted such that $t_1 < \cdots < t_N$. The synaptic inputs to the neuron are sorted as well into vector $\mathbf{s_i} = (s_i(1), s_i(2), \ldots, s_i(N))$, such that $s_i(1) < s_i(2) < \cdots < s_i(N)$.

Given an invertible transfer function, the targets can now be propagated back through the hidden layer, and a linear model can be defined that maps the sorted $s_i(k)$ as closely as possible to the sorted t_k. To this end, a model $\Phi(\mathbf{s}_i) = (\mathbf{s}_i^T, (1 \ldots 1)^T)$ and parameter vector $\mathbf{v}_i = (a_i, b_i)^T$ are defined. Then, given the invertible transfer function f the optimal slope a_i and bias b_i for which each $s_i(k)$ is approximately mapped to t_k can be found by minimizing

$$||\Phi(\mathbf{s}_i) \cdot \mathbf{v}_i - f^{-1}(\mathbf{t})||$$

The optimal slope a_i and bias b_i can therefore, like in ELM, be determined using the Moore-Penrose pseudo-inverse:

$$\mathbf{v}_i = (a_i, b_i)^T = \Phi^{\dagger}(\mathbf{s}_i) \cdot f^{-1}(\mathbf{t})$$

This procedure is performed for every neuron with an invertible transfer function, and even though the target distribution can often not exactly be matched (due to the limited degrees of freedom in the optimization problem) it has been shown in (Neumann and Steil, 2011, 2013; Neumann, 2013) that batch intrinsic plasticity is an effective and efficient scheme for input-specific tuning of input weights and biases used in the non-linear transfer functions.

The stability of BIP-ELM combined with ridge regression like in the R-ELM (Deng et al., 2009) essentially removes the need to tune the amount of hidden neurons, and the only parameter of batch intrinsic plasticity is the mean of the exponential target distribution from which targets $\mathbf{t}$ are drawn, which is either set to a fixed value c, or randomly in the interval $[0, 1]$ on a per-neuron basis (Neumann and Steil, 2011, 2013; Neumann, 2013). These variants will be referred to as BIP(c)-ELM and BIP(rand)-ELM in this thesis.

3.5 Other ELM approaches

Besides the above-mentioned approaches, several other approaches have been developed over the past years, extending the ELM framework to different types of models, namely kernelized ELM (Frénay and Verleysen, 2010, 2011; Huang et al., 2010; Parviainen et al., 2010), multiple kernel ELM (Liu et al., 2015), representation learning using ELM (Kasun et al., 2013), ELMs with shaped input weights (Tapson et al., 2014; McDonnell et al., 2014), and semi-supervised and unsupervised ELM (Huang et al., 2014). More details on these methods can be found in the cited references, or in (Huang et al., 2015).

Furthermore, randomization ideas akin to ELM are increasingly being used in modern kernel methods, in order to let them scale to larger data, namely Random Kitchen Sinks (Rahimi and Recht, 2007, 2008), and Fastfood (Le et al., 2013).

3.6 ELM in practice

In theory, random initialization of the hidden layer and use of any non-constant piecewise continuous transfer function is sufficient for approximating any function, given enough neurons. In practice, however, there are a number of practical strategies that can be used for obtaining more accurate and effective ELMs. This section lists some of those practical tips for building a more effective ELM.

Normalization and pre-training As is well-known, data should be normalized such that each variable is zero-mean and unit-variance (or scaled to e.g. interval $[-1, 1]$. In practice, the former approach is more robust, since it is not as sensitive to outliers.

The range and number of input variables, together with the random weights of an ELM, will result in an expected activation at the input of each neuron, and one should make sure that e.g. the sigmoid neuron is not always operating in the saturated or linear region. For example, by letting the parameters of the probability distribution from which the random layer weights and biases are drawn depend on the number of inputs and transfer function, or by cross-validating them to optimize accuracy.

Another fast option is to use the Batch-Intrinsic Plasticity pre-training from Section 3.4.4, which automatically adapts the randomly drawn hidden layer weights and biases, such that each neuron operates in a useful

regime.

Approximating the constant component In the non-kernel version of ELM, it might be helpful to include a bias in the output layer (i.e. achieved by concatenating the $\mathbf{H}$ matrix with a column of ones). Although this output bias is often not included in the description of the ELM since theoretically it is not needed, it allows the ELM to adapt to any non-zero mean in the targets at the expense of only a single extra parameter, namely the extra output weight.

Approximating the linear component Furthermore, in most problems, it is helpful to include a linear neuron for each input variable. This way, the rest of the nonlinear neurons can focus on fitting the nonlinear part of the problem, while the linear neurons take care of the linear part of the problem. Equivalently, an ELM could be trained on the residual of a linear model. This approach of decomposing the problem into a linear part and a nonlinear part has proven to be very effective in the context of deep learning (Raiko and Valpola, 2012).

4. Ensemble learning

"The only way of discovering the limits of the possible is to venture a little way past them into the impossible."

– Arthur C. Clarke

When discussing ensemble models it is helpful to look at a real-world example first. At fairs and exhibitions, sometimes there are these contests where the goal is to guess the number of marbles in a vase, and the person who makes the best guess wins the price. It turns out that while each individual guess is likely to be pretty far off, the average of all guesses is often a relatively good estimate of the real number of marbles in the vase. This phenomenon is often referred to as 'wisdom of the crowds'.

A similar strategy is employed in ensemble models: a number of individual models is built to solve a particular task, and these models are then combined into an ensemble model. Although the individual models might vary a lot in terms of accuracy, the combination gives a more accurate result.

This chapter introduces ensemble models, and the ELM-based ensemble models developed in this thesis, which make the ensemble adaptive to changes in the environment (Publication I) and allow them to scale to larger data (Publication II).

4.1 Ensemble Models

An ensemble model or committee (Bishop, 2006), combines multiple individual models, with the goal of reducing the expected error of the model. Commonly, this is done by taking the average or a weighted average of the individual models (see Figure 4.1).

Ensemble methods rely on having multiple good models with sufficiently uncorrelated errors. The simplest way to build an ensemble model is to

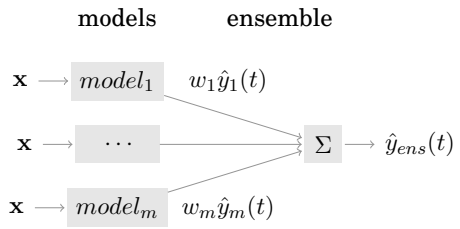


Figure 4.1. A schematic overview of how models can be combined in an ensemble (van Heeswijk, 2009)

take the average of the individual models (e.g. Figure 4.1, with $w_1 = \cdots = w_m = \frac{1}{m}$). In this case the output of the ensemble model becomes:

$$\hat{y}_{ens} = \frac{1}{m}\sum_{i=1}^{m}\hat{y}_i, \tag{4.1}$$

where $\hat{y}_{ens}$ is the output of the ensemble model, $\hat{y}_i$ are the outputs of the individual models and m is the number of models.

Now, following (Bishop, 2006), and assuming that the models are unbiased (i.e. absolute errors are zero-mean) and make independent errors, it can be shown that the variance of the ensemble model is lower than the average variance of all the individual models.

4.1.1 Error reduction by taking simple average of models

Suppose y denotes the true output to predict and $\hat{y}_i$ is the estimation of model i for this value. Then, the output $\hat{y}_i$ of model i can be written as the true value y plus some error term ϵ_i

$$\hat{y}_i = y + \epsilon_i, \tag{4.2}$$

and the expected error of the model is simply the mean square error

$$\mathbb{E}[\{\hat{y}_i - y\}^2] = \mathbb{E}[\epsilon_i^2]. \tag{4.3}$$

Now, define the average mean square error made by the models by

$$E_{avg} = \frac{1}{m}\sum_{i=1}^{m}\mathbb{E}[\epsilon_i^2]. \tag{4.4}$$

Similarly, define the expected error of the ensemble as defined in Equation 4.1 by

$$E_{ens} = \mathbb{E}\Big[\Big\{\frac{1}{m}\sum_{i=1}^{m}(\hat{y} - y)\Big\}^2\Big] = \mathbb{E}\Big[\Big\{\frac{1}{m}\sum_{i=1}^{m}\epsilon_i\Big\}^2\Big]. \tag{4.5}$$

Then, assuming the errors ϵ_i are uncorrelated (i.e. $\mathbb{E}[\epsilon_i \epsilon_j] = 0$) and are zero-mean (i.e. $\mathbb{E}[\epsilon_i] = 0$), the expected ensemble error can be written as

$$E_{ens} = \frac{1}{m} E_{avg} = \frac{1}{m^2} \sum_{i=1}^{m} \mathbb{E}[\epsilon_i^2], \tag{4.6}$$

which suggests a great reduction of the error through ensembling. These equations assume completely uncorrelated errors between the models, while in practice errors tend to be highly correlated. Therefore, errors are often not reduced as much as suggested by these equations. It can be shown though that $E_{ens} < E_{avg}$ always holds (Bishop, 2006), so through ensembling, the test error of the ensemble is expected to be smaller than the average test error of the models.

Note however, that it is not a guarantee that the ensemble is more accurate than the best model in the ensemble, but only as accurate as the models, on average. Therefore, besides being as independent as possible, it is important that the models used to build the ensemble are sufficiently accurate.

4.1.2 Ensemble weight initialization

Besides taking a simple average of the models, it is also possible to take a weighted linear combination based on some criterion that measures the quality of the models.

Two different ensemble weight initializations are investigated in the publications in this thesis: uniform weight initialization (Publication I) and leave-one-out weight initialization (Publication II).

Uniform weight initialization For initialization of the ensemble model, each of the individual models is trained on a given training set, and initially each model contributes with the same weight to the output of the ensemble. This will be referred to as *uniform weight initialization*.

Leave-one-out weight initialization As an alternative to uniform weight initialization, the initial weights can be based on the leave-one-out output of the models on the training set, like in Breiman (1996b). This will be referred to as *leave-one-out weight initialization*.

Using Equation 2.9, for a any model that is linear in the parameters (like ELM), the leave-one-out errors can be efficiently computed. Therefore, the leave-one-out outputs (i.e. the estimations of the sample that is left out in each of the N folds) can be obtained efficiently as well, given the leave-one-out errors and the true targets.

Finally, the initial ensemble weights are obtained by fitting a non-negative linear combination of the leave-one-out outputs for all m models to the target outputs. Using this procedure, models that have bad generalization performance get relatively low weight, while models with good generalization performance get higher weights.

4.1.3 Ensembling strategies

It was shown in (Hansen and Salamon, 1990), that through combining multiple neural networks, accuracy can be improved as compared to the individual neural networks. Since, several strategies have been proposed for building ensembles. In *mixture of experts* (Jacobs et al., 1991), several models are built, each of which specializes on part of the problem domain. The weights of the ensemble model depend on the part of the domain in which a prediction is required. In *stacking* (Wolpert, 1992) and *boosting* (Freund and Schapire, 1996; Schapire et al., 1998), the models are built in sequence, taking into account the performance of the earlier built models, in order to improve on them. In bootstrap aggregating, or *bagging* (Breiman, 1996a), on the other hand, diversity between the models is obtained by training them on re-sampled versions of the training set, while in *stacked regressions* (Breiman, 1996b), leave-one-out cross-validation is used to obtain the ensemble weights. Finally, in (Liu and Yao, 1999) accuracy of a neural network ensemble is enhanced through negative correlation learning, which promotes diversity between the neural networks. For an overview of ensemble methods in general, see (Bishop, 2006; Murphy, 2012).

In the next section, adaptive ensemble models, and the contributions made in this thesis are discussed.

4.2 Adaptive ensemble models

When solving a particular regression or classification problem, it is often unknown in advance what the optimal model class and structure is. One alternative for selecting the optimal model class or structure would be through validation, cross-validation or leave-one-out validation, as discussed in Section 2.2.2. However, it is not guaranteed that the model selected based on a set of training samples will be the best model for newly

obtained samples. For example, in a nonstationary context where the i.i.d. assumption does not hold and the information gathered from past samples can become inaccurate.

One strategy for handling nonstationarities would be to keep learning as new samples become available. For example, by retraining the model repeatedly on a finite window into the past such that it 'tracks' the nonstationarity.

Another strategy for adapting to nonstationarities is to use a strategy similar to (Jacobs et al., 1991), but instead of letting the linear combination of models depend on the part of the input space, let the linear combination directly depend on the accuracy of the models.

4.2.1 Adaptive ensemble model of ELMs

In Publication I, both strategies are investigated in one-step ahead prediction on both stationary and nonstationary time series, in which the next value of the time series is predicted, given all its past values.

Besides the already mentioned advantages of ensemble models over single models, this allows for adaptivity of the ensemble model to environmental changes.

Related Work The retraining of the ELMs in this ensemble is similar to the Online Sequential ELM (OS-ELM) (Liang et al., 2006), the important difference being that contrary to OS-ELMs, Publication I also provides a way to incrementally remove samples from the trained model. Furthermore, compared to the ensemble of OS-ELM (EOS-ELM) (Lan et al., 2009), which was introduced around the same time as Publication I, the adaptive ensemble adjusts the linear combination to optimize ensemble accuracy.

Both the ability to train on sliding windows, and the adaptive ensemble weights turn out to be an important contribution in the nonstationary environments, in which online sequential learning is typically applied.

Initializing the adaptive ensemble model The adaptive ensemble model consists of a number of randomly generated ELMs, which each have their own parameters. Because of the stochastic nature of the ELM, they are diverse in nature and will have different biases and input layer weights. To further increase diversity between the models, each ELM is built using different regressor variables; different regressor size; and different number of hidden neurons. Uniform weight initialization is used for the

Algorithm 3 Adaptive Ensemble of ELMs (Publication I)

Given $(\mathbf{x}(t), y(t))$, $\mathbf{x}(t) \in \mathbb{R}^d$, $y(t) \in \mathbb{R}$, and m models:

Create and train m random ELMs: $(ELM_1 \dots ELM_m)$
Initialize each w_i to $\frac{1}{m}$
while $t < t_{end}$ **do**
  generate predictions $\hat{y}_i(t+1)$
  $\hat{y}_{ens}(t+1) = \sum_i w_i \hat{y}_i(t+1)$
  t = t + 1
  compute all errors $\rightarrow \epsilon_i(t-1) = \hat{y}_i(t-1) - y(t-1)$
  for i = 1 to #models **do**
    $\Delta w_i = -\epsilon_i(t-1)^2 + mean(\epsilon(t-1)^2)$
    $\Delta w_i = \Delta w_i \cdot \alpha / (\#models \cdot \mathbf{var}(y))$
    $w_i = \max(0, w_i + \Delta w_i)$
    Retrain ELM_i
  end for
  renormalize weights $\rightarrow \mathbf{w} = \mathbf{w} / ||\mathbf{w}||$
end while

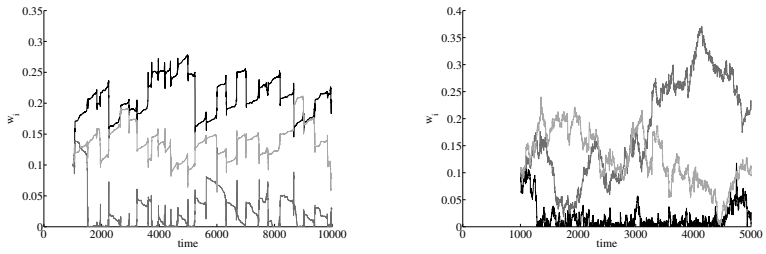
ensemble weights.

Adapting the linear combination of models On the one hand, a number of different models are combined in a single ensemble model and the weights with which these models contribute to the ensemble are adapted based on their performance (see Algorithm 3 for details). The speed of the change can be controlled by a learning rate α.

The idea behind the algorithm is that as the time series changes, a different model will be more optimal to use in prediction. By monitoring the errors that the individual models in the ensemble make, a higher weight can be given to the models that have good prediction performance for the current part of the time series, and a lower weight can be given to the models that have bad prediction performance for the current part of the time series.

Figure 4.2 illustrates the resulting adaptation of the ensemble weights, during the task of one-step ahead prediction on two different time series.

Retraining the models On the other hand, Publication I explores the effect of different ways of retraining the models as new data becomes available: before making a prediction for time step t, each model is either retrained on a past window of n values $(\mathbf{x}_i, y_i)_{t-n}^{t-1}$ (sliding window), or on all values known so far $(\mathbf{x}_i, y_i)_1^{t-1}$ (growing window), using the recursive



(a) **(b)**

Figure 4.2. Plots showing part of the ensemble weights w_i adapting over time during sequential prediction on (a) Laser time series and (b) Quebec Births time series (learning rate=0.1, number of models=10) (Publication I)

least-squares algorithm as defined by (Bierman, 1977; Bontempi et al., 1998).

Through this algorithm samples can be incrementally added to an already trained linear model, which will result in the linear model that would have been obtained, had it been trained on the modified training set. Since an ELM is essentially a linear model of the responses of the hidden layer, it can be applied to (re)train the ELM quickly in an incremental way on a sliding window or a growing window and it can adapt.

Adding a sample to a linear model Suppose a linear model is trained on k samples of dimension d, with solution $\boldsymbol{\beta}(k)$, and have $\mathbf{P}(k) = (\mathbf{X}^T\mathbf{X})^{-1}$, which is the $d \times d$ inverse of the covariance matrix based on k samples, then the solution of the model with added sample $(\mathbf{x}(k+1), y(k+1))$ can be obtained by

$$\begin{aligned}
&\mathbf{P}(k+1) = \mathbf{P}(k) - \tfrac{\mathbf{P}(k)\mathbf{x}(k+1)\mathbf{x}^T(k+1)\mathbf{P}(k)}{1+\mathbf{x}^T(k+1)\mathbf{P}(k)\mathbf{x}(k+1)},\\
&\gamma(k+1) = \mathbf{P}(k+1)\mathbf{x}(k+1),\\
&\varepsilon(k+1) = y(k+1) - \mathbf{x}^T(k+1)\hat{\boldsymbol{\beta}}(k),\\
&\hat{\boldsymbol{\beta}}(k+1) = \hat{\boldsymbol{\beta}}(k) + \gamma(k+1)\varepsilon(k+1)
\end{aligned} \tag{4.7}$$

where $\mathbf{x}(k+1)$ is a $1 \times d$ vector of input values, $\boldsymbol{\beta}(k+1)$ is the solution to the new model and $\mathbf{P}(k+1)$ is the new inverse of the covariance matrix on the $k+1$ samples (Bierman, 1977; Bontempi et al., 1998).

Removing a sample from a linear model Similarly, a sample can be removed from the training set of a linear model giving the linear model that would have been obtained, had it been trained on the modified training set. In this case, the new model with removed sample $(\mathbf{x}(k), y(k))$ can be obtained by

$$
\begin{aligned}
&\gamma(k-1) = \mathbf{P}(k)\mathbf{x}(k), \\
&\varepsilon(k-1) = y(k) - \tfrac{\mathbf{x}(k)\hat{\boldsymbol{\beta}}(k)}{1-\mathbf{x}^T(k)\mathbf{P}(k)\mathbf{x}(k)}, \\
&\mathbf{P}(k-1) = \mathbf{P}(k) - \tfrac{\mathbf{P}(k)\mathbf{x}(k)\mathbf{x}^T(k)\mathbf{P}(k)}{1+\mathbf{x}^T(k)\mathbf{P}(k)\mathbf{x}(k)}, \\
&\hat{\boldsymbol{\beta}}(k-1) = \hat{\boldsymbol{\beta}}(k) - \gamma(k)\varepsilon(k)
\end{aligned}
\tag{4.8}
$$

where $\boldsymbol{\beta}(k-1)$ is the solution to the new model and $\mathbf{P}(k-1)$ is the new inverse of the covariance matrix on the $k-1$ samples (Bierman, 1977; Bontempi et al., 1998; van Heeswijk, 2009).

4.2.2 Experiments

In the experiments of Publication I, the adaptive ensemble model of Extreme Learning Machines (ELMs) is applied to the problem of one-step ahead prediction on both stationary and nonstationary time series. It is verified that the method works on stationary time series, and the adaptivity of the ensemble model is verified on nonstationary time series.

Data The stationary data used in the experiments is the Santa Fe Laser Data time series (Weigend and Gershenfeld, 1993), which has been obtained from a far-infrared-laser in a chaotic state. This time series has become a well-known benchmark in time series prediction since the Santa Fe competition in 1991. It consists of approximately 10000 points. The non-stationary data used in the experiments is The Quebec Births time series[1], which records the number of daily births in Quebec over the period of January 1, 1977 to December 31, 1990. It consists of approximately 5000 points, is nonstationary and more noisy than the Santa Fe Laser Data.

Experimental parameters The adaptive ensemble model is trained on the first 1000 values of the time series, after which sequential one-step ahead prediction is performed on remaining values. This experiment is repeated for various combinations of learning rate α and number of models in the ensemble. Each ELM has a regressor size (of which a number of variables are randomly selected) and between 150 and 200 hidden neurons with a sigmoid transfer function. See Publication I for more details.

Effect of number of models and learning rate on accuracy

[1] `http://www-personal.buseco.monash.edu.au/~hyndman/TSDL/misc/qbirths.dat`

Stationary data Figure 4.3 shows the effect of the number of models and the learning rate, which controls how quickly the ensemble weights adapt, on the prediction accuracy in the stationary case. It can be seen that the number of models strongly influences the prediction accuracy and that at least 40 models are needed to get good prediction accuracy. Furthermore, despite the data being stationary, it can be seen that a non-zero learning rate helps in adapting the linear combination of the models for optimal performance, presumably because the uniform initialization of the ensemble weights is sub-optimal.

Nonstationary data Figure 4.4 shows the effect of the number of models and the learning rate on the prediction accuracy in the nonstationary case. Again, it can be seen that the number of models strongly influences the prediction accuracy and that, compared to the stationary case, more models are needed to get good prediction accuracy.

Effect of retraining strategy on accuracy The influence of the various (re)training strategies can be found in Table 4.1.

As is to be expected, for the stationary data, optimal results are obtained for retraining on a growing window. For the nonstationary data, as expected, a sliding window is optimal.

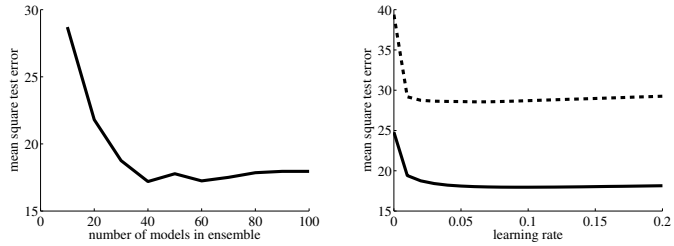
Discussion In general, the results of Publication I suggest the following strategy for obtaining robust models:

1. the more models are included in the ensemble, the more accurate it generally is (although there are diminishing returns).

2. a small learning rate of around 0.1 is optimal.

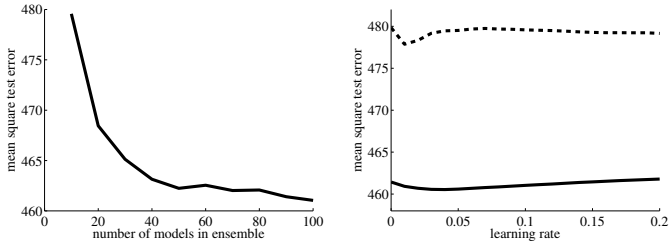
3. individual models should be retrained according to expectations/expertise.

The retraining strategy of the individual models affects the accuracy and often it is not known whether data is stationary or nonstationary, nor is the optimal sliding window size known. Future work could therefore include the investigation of ensembles consisting of models with varying retraining strategies and window sizes. Furthermore, to save computational resources, models that contribute little to the accuracy of the ensemble could be pruned. Vice versa, new models could be added to the ensemble when needed.



(a) **(b)**

Figure 4.3. MSE_{test} of ensemble on **Santa Fe Laser Data** time series for varying number of models (no window retraining, learning rate 0.1), and as a function of learning rate (no window retraining), for 10 models (*dotted line*) and 100 models (*solid line*)



(a) **(b)**

Figure 4.4. MSE_{test} of ensemble on **Quebec births** time series for varying number of models (no window retraining, learning rate 0.1), and as a function of learning rate (no window retraining), for 10 models (*dotted line*) and 100 models (*solid line*)

		retraining		
	learning rate	none	sliding	growing
laser	0.0	24.80	33.85	20.99
	0.1	17.96	27.30	**14.64**
qbirths	0.0	585.53	**461.44**	469.79
	0.1	567.62	**461.04**	468.51

Table 4.1. MSE_{test} of ensemble of 100 ELMs for laser (training window size 1000)

4.3 GPU-accelerated and parallelized ELM ensembles

A big advantage of ensemble models is their modularity. Publication II exploits this modularity of ensembles and presents an ensemble of GPU-accelerated ELMs, that is accelerated in three distinct ways:

1. multiple individual models are trained in parallel across multiple graphics processor units (GPUs) and CPU cores.

2. the training and model structure selection procedures are accelerated by using the GPU.

3. the model structure selection is performed in an efficient way by use of PRESS statistics, while explicitly computing and reusing the pseudo-inverse of $\mathbf{H}^{\dagger}$, where $\mathbf{H}$is the hidden layer output matrix.

Experiments show that competitive performance is obtained on the regression tasks, and that the GPU-accelerated and parallelized ELM ensemble achieves attractive speedups over using a single CPU. Furthermore, the proposed approach is not limited to a specific type of ELM and can be employed for a large variety of ELMs. The next sections will highlight the contributions and experimental results of Publication II.

4.3.1 Parallelization across multiple cores

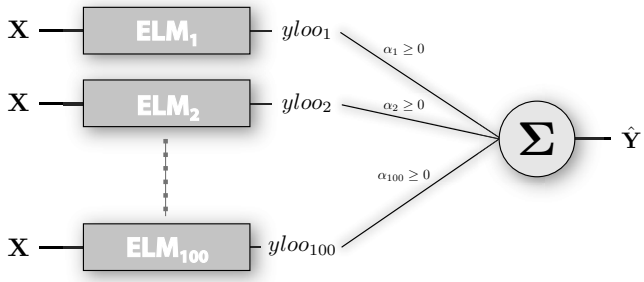


Figure 4.5. Block diagram showing the overall setup of the ensemble of ELMs. (Publication II)

Figure 4.5 illustrates the ELM ensemble of Publication II, and it can be seen that the ELMs in the ensemble can be built independently. Therefore, the running time of the ensemble can be optimized by dividing the

ELMs across multiple CPUs and GPUs and preparing them in parallel. This is achieved using MATLAB's Parallel Computing Toolbox (MathWorks, 2011), which allows the creation of a pool of so-called MATLAB workers. Each of the workers runs its own thread for executing the program, and gets its own dedicated GPU assigned to it, which is used to accelerate the training and model structure selection that has to be performed for each model. As an example, in case of an ensemble of 100 ELMs and 4 workers, each of the workers builds 25 ELMs.

Although in Publication II the parallelized ensemble model was not executed across multiple computers, it can be executed on multiple computers by using the MATLAB Distributed Computing Toolbox, for which at the time of writing Publication II no license was available.

4.3.2 GPU-acceleration of required linear algebra operations

Since the running time of the ELM algorithm largely consists of a single operation (solving the linear system), it is the prime target for optimizing the running time of the ELM. If this operation can be accelerated, then the running time of each ELM (and thus of the ensemble) can be greatly reduced. In this work, this operation is performed on the GPU.

Available libraries There exist several software libraries aimed at speeding up a subset of the linear algebra functions found in LAPACK (Anderson et al., 1999):

- CULA Tools (Humphrey et al., 2010): a library introduced in October 2009, implementing a subset of LAPACK functions. It was the first widely available GPU-accelerated linear algebra package, and developed in cooperation with NVidia. Because of NVidia's investment in general-purpose GPU computing, this library is likely to remain well-supported. The free variant of this package contains functions for solving a linear system (`culaGesv`), and for computing the least-squares solution to a linear system (`culaGels`).

- MAGMA (Agullo et al., 2009): a linear algebra package, developed by the creators of the widely used LAPACK, aiming at running linear algebra operations on heterogeneous architectures (i.e. using both multicore CPU and multiple GPUs present on the system, in order to solve a single problem).

function name	description	runs on
`mldivide`	solve linear system (MATLAB)	CPU
`gesv`	solve linear system (LAPACK)	CPU
`gels`	least-square solve (LAPACK)	CPU
`culaGesv`	solve linear system (CULA)	GPU
`culaGels`	least-square solve (CULA)	GPU

Table 4.2. An overview of the various functions used. (Publication II)

Solving linear systems on CPU vs GPU In Publication II, CULA Tools is used for accelerating the linear algebra operations. Specifically, the (`culaGesv`) and (`culaGels`) functions are used, and wrappers around these functions were written, such that they can be used from MATLAB in the training and model structure selection of the ELM. Similar functions are offered by MATLAB and its underlying LAPACK library.

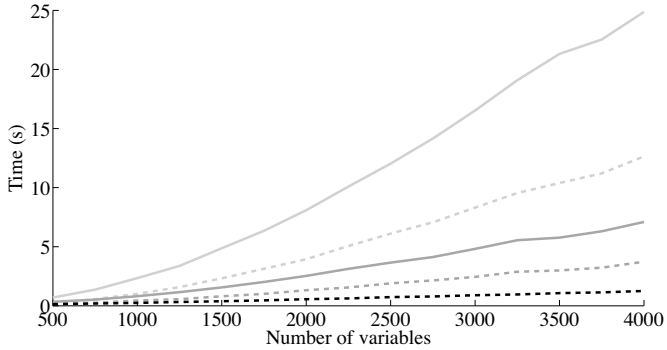
Relevant functions An overview of all the functions used in Publication II can be found in Table 4.2. Since in Publication II all linear systems are fully determined, and involve square regressor matrices, the functions give exactly the same result and only vary in running time.

Single vs. double-precision Even though double-precision calculations are possible on GPU, they are faster at performing single-precision calculations. In particular, for the NVidia GTX295 cards that were used in Publication II, the single-precision performance is 8 times higher than the double-precision performance. In NVidia's latest generation of video cards, this gap in performance is smaller, but still existent. Therefore, it is beneficial to use single-precision calculations wherever numerically possible.

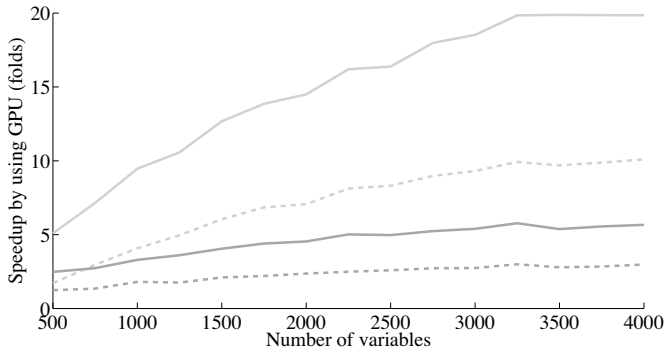
Performance comparison In order to get an idea of the running time of the function `culaGels`, it is compared with MATLAB's commonly used `mldivide` (also known as \), as well as with the `gels` function from MATLAB's underlying highly optimized multi-threaded LAPACK library[2]. For a fair comparison, and since on the CPU the performance in single-precision is about twice the double-precision performance, the functions are compared in both single-precision and double-precision.

Figure 4.6a and Figure 4.6b summarize the results. As expected, it can be seen that the precision greatly affects the performance. Also, MAT-

[2]MATLAB r2009b was used, which utilizes the highly optimized MKL library by Intel on the Core i7 920 used for the experiments.



(a) Time (s) needed to solve linear system in double-precision (*solid lines*) and single-precision (*dashed lines*).



(b) Speedup of `culaGels` over other functions in double-precision (*solid lines*) and single-precision (*dashed lines*).

Figure 4.6. Performance comparison of functions for solving a linear system of 5000 samples and one target variable: `mldivide` (*light-gray lines*), `gels` (*gray lines*), `culaGels` (*black line*) (Publication II).

LAB's underlying LAPACK function `gels` perform much better than the commonly used `mldivide`. Finally, the GPU-accelerated function `culaGels` offers the fastest performance of all.

Finally, for square matrices, `culaGesv` and `gesv` (not pictured) are slightly faster than `gels` and `culaGels` and are therefore used in Publication II for slightly higher performance.

4.3.3 Efficient leave-one-out computation

Model structure selection allows for determining the optimal structure for the ELM model, where by optimal structure often the number of hidden neurons is meant. Besides the number of hidden neurons, also other parameters of the ELM and the used training algorithm can be cross-validated this way. This is done using a criterion which estimates the

model generalization capabilities for the varying numbers of neurons in the hidden layer and the different other possible values for model parameters considered.

Minimal overhead in LOO computation by re-using pseudo-inverse Recall from Equation 2.9, that the HAT matrix needed in the computation of the leave-one-out error largely consists of the Moore-Penrose generalized inverse of the regressor matrix. Using the notations of ELM, HAT $= \mathbf{H}\mathbf{H}^{\dagger}$. Therefore, instead of just computing the solution to the linear system while training the ELM, combined training and leave-one-out computation can be optimized by using a method that explicitly computes $\mathbf{H}^{\dagger}$. The $\mathbf{H}^{\dagger}$ computed during training can then be reused in the computation of the leave-one-out error.

Furthermore, since only the diagonal of the HAT-matrix is needed, it is sufficient to compute only the diagonal by taking the row-wise dot-product between $\mathbf{H}$ and $\mathbf{H}^{\dagger T}$, and it is not needed to compute $\mathbf{H}\mathbf{H}^{\dagger}$ in full. Therefore, the computation of the leave-one-out error then comes at a very low overhead once the pseudo-inverse is already computed.

Figure 4.7 illustrates this by comparing the running times for training and combined training and leave-one-out computation. It can be seen that although by explicitly computing $\mathbf{H}^{\dagger}$, the training procedure becomes somewhat slower, due to the re-use of $\mathbf{H}^{\dagger}$ in the leave-one-out-computation, combined training and leave-one-out computation can be done about as fast as just training the model.

Incidentally, because leave-one-out cross-validation virtually comes for free after training, it is a great alternative to using information criteria like AIC (Akaike, 1974) and BIC (Schwarz, 1978), which are often used in situations where cross-validation would be prohibitively slow.

The algorithm for fast training and leave-one-out-based model structure selection of ELM can then be summarized as in Algorithm 4. Although this particular example is for cross-validating the number of hidden neurons, the same approach can be used when cross-validating for other combinations of model parameters. Also, in case the neurons would be sorted by relevance first, the algorithm corresponds to OP-ELM (Miche et al., 2010). In case also an L2-regularization parameter is optimized at each number of neurons considered, this corresponds to TROP-ELM (Miche et al., 2011).

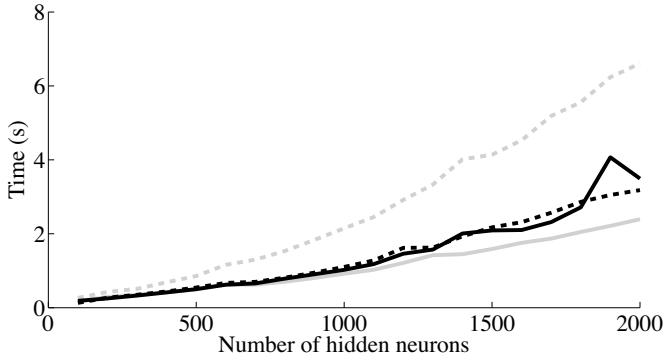


Figure 4.7. Comparison of running times of ELM training (*solid lines*) and ELM training + leave-one-out-computation (*dotted lines*), with (*black lines*) and without (*gray lines*) explicitly computing and reusing $\mathbf{H}^\dagger$ (Publication II)

Algorithm 4 Efficient LOO cross-validation of the number of neurons for an ELM (Publication II)

Given a training set $(\mathbf{x}_i, y_i), \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$, an activation function $f : \mathbb{R} \mapsto \mathbb{R}$ and $\aleph = \{n_1, n_2, \ldots, n_{max}\}$ defining set of possible numbers of hidden neurons.

1: Generate the weights for the largest ELM:
2: - Randomly generate input weights $\mathbf{w}_i$ and biases b_i, $i \in [1, n_{max}]$;
3: **for** all $n_j \in \aleph$ **do**
4: Train the ELM:
5: - Given the input weights and biases for the first n_j neurons;
6: - Calculate the hidden layer output matrix $\mathbf{H}$;
7: - Calculate $\mathbf{H}^\dagger$ by solving it from $(\mathbf{H}^T\mathbf{H})\mathbf{H}^\dagger = \mathbf{H}^T$;
8: - Calculate output weights matrix $\boldsymbol{\beta} = \mathbf{H}^\dagger\mathbf{Y}$;
9: Compute E_{loo}:
10: - Compute $\mathrm{diag}(\mathrm{HAT})$ (row-wise dot-product of $\mathbf{H}$ and $\mathbf{H}^{\dagger T}$);
11: - $E_{loo,j} = \frac{1}{M}\sum_{i=1}^{M}\frac{y_i - \hat{y}_i}{1 - hat_{ii}}$;
12: **end for**
13: As model structure, select the ELM with that number of hidden neurons $n_j \in \aleph$, which minimizes $E_{loo,j}$;

4.3.4 Experiments

In Publication II, an ensemble model of ELMs is built for solving two relatively large regression problems based on one-step-ahead time series prediction. The model structure selection and training of the ELMs is accelerated using GPU, and the construction of the ensemble is parallelized

by distributing the work over multiple CPUs and GPUs. The influence of the GPU-acceleration and parallelization is measured, and scalability of the approach is verified on two data sets.

Data The first data set is again the Santa Fe Laser Data time series (Weigend and Gershenfeld, 1993), which consists of approximately 10000 samples.

The second data set is the ESTSP'08 Competition data set number 3[3], which consists of approximately 30000 samples, and is computationally also more challenging due to the size of the regressor needed (Olteanu, 2008; Kourentzes and Crone, 2008).

Experimental parameters The samples from the time series are obtained using respectively 12, and 168 time steps for the Santa Fe Laser data and ESTSP'08 Competition data, after which the data is randomly divided into 85% for training and 15% for testing.

The ELMs have their number of neurons optimized using efficient leave-one-out cross-validation and for diversity, each ELM uses random variables from the regressor. The ensemble weights are determined through leave-one-out initialization and remain fixed.

The effect of GPU-acceleration and parallelization on the performance is consequently measured by varying the function used in model structure selection and training, as well as varying the number of MATLAB workers (i.e. threads). See Publication II for more details.

Effect of GPU-acceleration and used function Table 4.3 summarizes the results of the experiments performed in Publication II, and clearly shows the effect of the GPU-acceleration and the used function.

It can be seen that generally `mldiv` and `gesv` achieve similar performances, while both the use of single-precision and the use of GPU significantly speed up the ensemble.

Effect of number of workers on computational time Table 4.3 and Figure 4.8 summarize the influence of the number of MATLAB workers on the ensemble performance.

When not using any explicit parallelization through MATLAB workers (i.e. the line $N = 0$ in Table 4.3), the differences between using CPU and GPU are relatively modest. This is due to the fact that for `mldiv` and `gesv`, MATLAB automatically parallelizes the computation over the

[3]available from `http://research.ics.aalto.fi/eiml/datasets.shtml`

multiple CPU cores of the Intel Core i7 920, and can therefore keep up quite well with the single GPU being used for `culaGesv`.

However, when explicitly parallelizing the computation over N cores and GPUs, the difference between CPU and GPU significantly increases.

Overall, the experiments show a 3.3 times speedup over the typical double-precision implementation of an ensemble of ELMs, by using the GPU to speed up the slowest part of the algorithm, and parallelizing across multiple CPU cores and GPUs (i.e. t($\texttt{mldiv}_{dp}$) / t($\texttt{culaGesv}_{sp}$)).

Effect of number of models on accuracy Finally, Figure 4.9 shows the influence of the number of models in the ensemble on the accuracy of the ensemble. Similarly to Publication I, the results show that the more models are added to the ensemble, the more accurate it gets.

Discussion This fact alone (that more models is generally better in ensemble models), is additional justification for the approach proposed in Publication II. By parallelization and GPU-acceleration of the ensemble, it is possible to train more models and to train them faster, which results in a more accurate model that can be obtained in less time.

Some interesting questions to explore therefore would be: how fast can an ensemble model of a particular accuracy be obtained? Of course the easiest way to speed up the ensemble would be to evaluate each model on its own dedicated node, but even then, would it be possible to further speed up the ensemble model while retaining or improving accuracy?

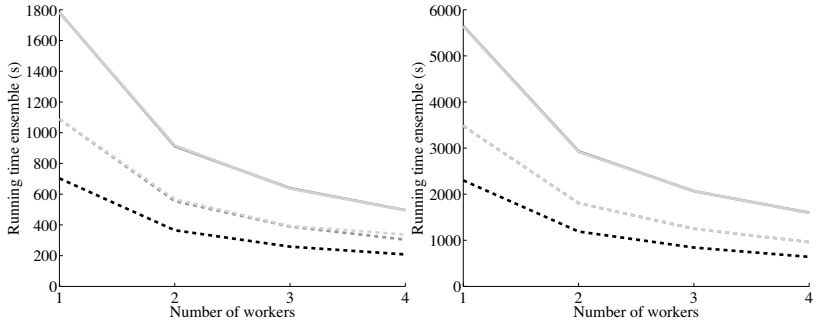
One possibility would be to parallelize other parts of the ELM, like the multiplication of the hidden layer weights and the inputs, as has been done in (He et al., 2011) and (He et al., 2013).

Another interesting direction to explore would be to make the ELMs more effective and accurate by an altered weight scheme (which is explored in Publication V), or by trading off speed for accuracy in the individual ELMs (which is explored in Publication VI) and ensembling more of them.

Before giving an overview of those publications though, the next chapter will highlight some contributions of the thesis to variable selection.

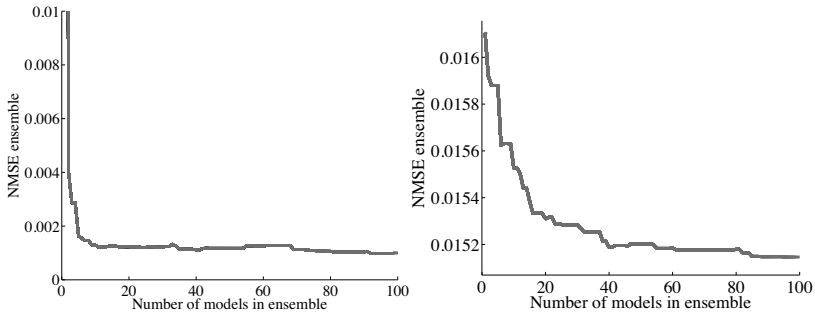
	N	t(mldiv$_{dp}$)	t(gesv$_{dp}$)	t(mldiv$_{sp}$)	t(gesv$_{sp}$)	t(culaGesv$_{sp}$)
SantaFe	0	674.0 s	672.3 s	515.8 s	418.4 s	401.0 s
	1	1781.6 s	1782.4 s	1089.3 s	1088.8 s	702.9 s
	2	917.5 s	911.5 s	567.5 s	554.7 s	365.3 s
	3	636.1 s	639.0 s	392.2 s	389.3 s	258.7 s
	4	495.7 s	495.7 s	337.3 s	304.0 s	**207.8 s**
ESTSP	0	2145.8 s	2127.6 s	1425.8 s	1414.3 s	1304.6 s
	1	5636.9 s	5648.9 s	3488.6 s	3479.8 s	2299.8 s
	2	2917.3 s	2929.6 s	1801.9 s	1806.4 s	1189.2 s
	3	2069.4 s	2065.4 s	1255.9 s	1248.6 s	841.9 s
	4	1590.7 s	1596.8 s	961.7 s	961.5 s	**639.8 s**

Table 4.3. Results for both data sets: Running times (in seconds) for running the entire ensemble in parallel on N workers, using the various functions in single-precision (sp) and double-precision (dp) (Publication II).



(a) **(b)**

Figure 4.8. Running times (in seconds) for running the entire ensemble in parallel on (a) Santa Fe, (b) ESTSP'08, for varying numbers of workers, using `mldivide` (*light-gray lines*), `gesv` (*gray lines*), `culaGesv` (*black line*) for double-precision (*solid lines*) and single-precision (*dashed lines*) (Publication II).



(a) **(b)**

Figure 4.9. NMSE of an ensemble model with varying number of models, on (a) Santa Fe, (b) ESTSP'08 (Publication II).

5. Variable Selection

"And what is good, Phaedrus,
And what is not good–
Need we ask anyone to tell us these things?"

– Robert M. Pirsig,
Zen and the Art of Motorcycle Maintenance

Variable selection is a central issue in machine learning. The higher the dimensionality of the data, the more samples are needed to reliably train a model. This is sometimes referred to as the curse of dimensionality. Therefore, given the often limited number of training samples, it is important that the dimensionality is sufficiently reduced (without losing too much information) such that a reliable model can be trained.

This chapter introduces the basic concepts of variable selection, and highlights the related contributions of this thesis: an ELM-based method for variable selection (Publication III); a (multi-)GPU-accelerated Delta Test criterion used as criterion in a parallelized genetic algorithm for variable selection (Publication IV); and finally, a new weight scheme for ELM that results in more effective and efficient neural networks, and makes the ELM more robust to irrelevant and noisy variables (Publication V).

5.1 Variable selection

5.1.1 Motivation

Due to the technological developments of the past decades, it is easier than ever to gather large amounts of data. The grand challenge, then, is to extract relevant information from this data in order to gain useful knowledge.

Part of that challenge is being able to scale the methods to the size of modern data sets (which was partly the focus of Chapter 4). However, besides challenges in scaling due to the large amount of samples in modern data sets, another challenge is posed by their high dimensionality. Namely, the high dimensionality of modern data sets poses a problem when trying to train reliable and accurate models due to the curse of dimensionality (Bellman, 1961; Verleysen et al., 2003): the number of samples required to be able to train an accurate model scales exponentially with the dimensionality of the input space (i.e. the dimensionality of the data). Therefore, it is important to reduce the dimensionality as much as possible, so that more accurate models may be trained.

5.1.2 Dimensionality reduction

Feature extraction Although the data is high-dimensional, it is often not evenly spread throughout the input space. Instead, the samples will lie on some lower-dimensional manifold embedded in that high-dimensional space. Therefore, one strategy for handling high-dimensional data is by dimensionality reduction through *feature extraction*. Here, the goal is to find an alternate representation of the data by extracting its latent features, and representing the data in terms of these features. For example, if the data lies linear in some linear subspace, then Principal Component Analysis (PCA) can be used to obtain a more compact representation (Jolliffe, 2002). Note however, that this by itself does not take into account the relevance of a latent feature for predicting the output, as it is unsupervised.

Variable selection Contrary to unsupervised feature extraction, v*ariable selection* (Guyon and Elisseeff, 2003) is supervised and does take into account the relevance of a variable for predicting the output[1]. Through a search algorithm, the variable subset is optimized according to a statistical criterion measuring the quality of the variable subset.

Besides improving model accuracy, another motivation for performing variable selection may be interpretability of the models and gaining a better understanding about the problem at hand. For example, in gene

[1]Of course, feature extraction and variable selection can be combined, and extracted features can become input variables to some model. In this work, it is assumed that feature extraction has already taken place, and the focus is on selecting the best variable subset, given a set of input variables. The terms variable selection and feature selection will be used interchangeably.

expression analysis, variable selection can help identifying those genes that are relevant for predicting whether a patient is sick, and are therefore likely to play a role in the disease itself (Guyon and Elisseeff, 2003).

Finally, sometimes it is very expensive to obtain new samples and measure particular variables. Therefore, through variable selection, money and effort can be saved by only measuring and collecting the most relevant variables.

5.1.3 Variable selection methods

Approaches Several main approaches for variable selection are distinguished in (Guyon and Elisseeff, 2003): wrapper methods, filter methods, and embedded methods, which will be described shortly below.

Filter approach In filter approaches, as the name suggests, the variable subset is filtered before being passed on to a model for learning, and some criterion is used to evaluate the quality of a particular subset of variables.

For example, as a criterion, mutual information (MacKay, 2003; Kraskov et al., 2004) can be used to estimate how much information a particular variable subset contains about the targets (Rossi et al., 2006; François et al., 2007; Verleysen et al., 2009). The mutual information criterion was used in the baseline variable selection experiments of Publication III.

Another criterion that can be used for variable selection is the Delta Test (Eirola et al., 2008; Eirola, 2014; Sovilj, 2014). The Delta Test is a noise variance estimator, which indicates the performance a non-linear model can possibly attain, given particular data. The Delta Test criterion was used in Publication IV.

As a final example, a filter method based on Least Angle Regression (LARS) (Efron et al., 2003) could rank the variables according to relevance, and return a subset of the most relevant variables. This approach is included in the baseline experiments of Publication III.

Wrapper approach Whereas filter strategies use some statistical criterion for variable selection, in the wrapper strategy, the model is used directly for evaluating the quality of a variable subset. For example, an Extreme Learning Machine could be built with many different variable subsets, and have its generalization performance estimated using fast leave-one-out cross-validation. The variable subset that achieves minimum leave-one-out error will then be used for building the final ELM. Therefore, it can be seen as some sort of model structure selection. The

advantage of wrapper strategies is that, since the actual model is used, the feature subset is likely to be better-optimized for that model. However, since the actual model needs to be trained, depending on the model, and the fact that there might not be a way to efficiently estimate the generalization performance, wrapper strategies can be computationally very expensive. Furthermore, care should be taken not to overfit during the feature selection process (Reunanen, 2003).

Embedded approach In the embedded approach, the learning machine itself incorporates variable selection as part of its training, and selection is not performed explicitly using a wrapper or filter approach. Although it could be argued that explicit variable selection in the training algorithm is actually model structure selection using a wrapper approach (rather than training and an embedded approach), it is useful to distinguish the embedded variable selection approach from filter and wrapper approaches, as the learning method might implicitly perform variable selection as a result of its structure (for example, like in the Binary ELM and Ternary ELM proposed in Publication V).

Search methods Besides a statistical criterion like mutual information, or an estimated performance of a model, a method is needed to explore the solution space of all possible variable selections in a systematic way, especially considering that the number of possible variable subsets is exponential in the number of variables.

One possibility is to use a local search method and, starting from a particular solution in the solution space, optimize the solution by repeatedly evaluating and jumping to neighboring candidate solutions, until an optimum is found. For example, Forward selection (Hastie et al., 2001) starts from an empty variable subset, and repeatedly adds the variable that improves the criterion the most. Similarly, Backward selection (Hastie et al., 2001) starts from the full variable subset, and repeatedly removes the variable that deteriorates the criterion the least. Finally, Forward-Backward selection allows both adding and removing variables at each step (Hastie et al., 2001). These local search methods are used in the baseline experiments of Publication III, in combination with the mutual information criterion.

Another possibility, which is explored in Publication IV, is to use a genetic algorithm to explore the space of possible solutions. Here, the candidate solutions are encoded in a population of individuals and consequently optimized through an evolution-like algorithm.

The remaining part of this chapter will give an overview of the contributions to variable selection methods that are made as part of this thesis.

5.2 ELM-FS: ELM-based feature selection

Publication III explores a feature selection method based on Extreme Learning Machine, which returns a complete feature selection path, representing the trade-off between the best feature subset for each subset size and the corresponding estimated generalization error. This allows the practitioner to make an informed decision about the feature subset that is best for the current context. For example, if sparsity is most important due to the difficulty of obtaining new samples, the smallest subset giving reasonable performance could be identified and selected. If, on the other hand, accuracy is more important, that feature subset giving best accuracy can be selected. The method is shown to be competitive with traditional feature selection methods, and can be used for ELM (as a wrapper method), or as an efficient filter method for more complicated non-linear machine learning methods.

5.2.1 Feature selection using the ELM

Introducing a scaling layer In order to use the Extreme Learning Machine for feature selection, it is first augmented with a scaling layer such that each input variable is multiplied with its own particular scale (i.e. for sample $\mathbf{x}_i$, $x_{i1} \rightarrow s_1 x_{i1}, \ldots, x_{id} \rightarrow s_d x_{id}$). Then, for regression, the feature selection problem for obtaining the feature subset that obtains minimum training error, can be written as

$$\min_{s,\theta} \frac{1}{n} \sum_{i=1}^{n} \left[y_i - f\left(s_1 x_{i1}, \ldots, s_d x_{id} | \theta \right) \right]^2 s.t. \left\| \mathbf{s} \right\|_0 \leq d \tag{5.1}$$

where $f\left(s_1 x_{i1}, \ldots, s_d x_{id} | \theta \right)$ stands for the ELM with parameters θ, and inputs $s_1 x_{i1}, \ldots, s_d x_{id}$. Here, the scaling vector s is a vector of binary variables such that $s_i \in \{0, 1\}$, and $\left\| s \right\|_0$ is the L_0-norm of s (i.e. the number of non-zero scaling factors and therefore the number of selected variables).

Now, Equation 5.1 can be rewritten as a regularization, i.e.

$$\min_{s,\theta} \frac{1}{n} \sum_{i=1}^{n} \left[y_i - f\left(s_1 x_{i1}, \ldots, s_d x_{id} | \theta \right) \right]^2 + C_0 \left\| s \right\|_0, \tag{5.2}$$

for some regularization constant C_0, that can be used to control the size

of the feature subset.

Relaxing the feature selection problem However, even though solving this optimization problem while gradually increasing C_0 would result in increasingly sparse optimal variable subsets, there are too many subsets to exhaustively evaluate all of them. Therefore, a common strategy in optimizing combinatorial problems is used. Namely, the feature selection problem is made easier through a technique known as relaxation (Burke and Kendall, 2005) and a regularization scheme is used to enforce sparsity: the binary scalings $s_i \in \{0, 1\}$ are replaced by real $\tilde{s}_i \in [0, 1]$, and the L_1-norm is used instead of the L_0-norm, which results in

$$\min_{\tilde{s},\theta} \frac{1}{n} \sum_{i=1}^{n} \left[t_i - f\left(\tilde{s}_1 x_{i1}, \ldots, \tilde{s}_d x_{id} | \theta\right)\right]^2 + C_1 \left\|\tilde{s}\right\|_1 . \tag{5.3}$$

This relaxed form of the optimization problem is easier to solve, since it is differentiable.

Solving the relaxed feature selection problem Since it is possible to obtain the gradient of the training error with respect to the scaling vector $\tilde{s}$, the algorithm can repeatedly take a small gradient descent step, updating $\tilde{s}$ such that the objective value of the optimization problem is improved. Therefore, for a given regularization parameter C_1, the problem can be efficiently solved.

However, there is the potential problem of plateaus where too small a step size would result in slow convergence towards the (local) optimum. Therefore, the scaling parameter $\tilde{s}$ is discretized and optimization of $\tilde{s}$ is performed on a hyper-grid instead. This guarantees termination of the algorithm, and limits the amount of steps the algorithm takes.

Now, optimal feature scalings of varying sparsity can be obtained by starting from a random initial $\tilde{s}$ and $C_1 = 0$, and repeatedly jumping to the neighbor pointed to by the gradient, until stuck in a local minimum.

At this point, the generalization error of that feature selection (each non-zero scaling indicating a feature being selected) can be estimated through fast leave-one-out error computation.

Obtaining a feature selection path and corresponding error estimates After getting stuck in a local optima, the regularization factor can be increased until the local minimum disappears, and minimization continues towards sparser scalings and eventually empty scalings.[2] Finally, by re-

[2]This sounds complicated, but it can be intuitively understood by seeing it as dropping a ball on a hilly landscape mountain, and letting it roll down. Whenever

peating this procedure many times and recording the optimal feature selections found for every feature subset size, a feature selection path, along with corresponding estimates of the generalization error is obtained. Algorithm 5 summarizes the full algorithm.

Algorithm 5 Local search algorithm for the relaxed feature selection problem (adapted from Publication III)

for all restarts **do**
  - $C_1 = 0$
  - initialize $\tilde{\mathrm{s}}$ randomly
  while $\tilde{\mathrm{s}} \neq 0$ **do**
    - estimate generalization error and update SET/FSP
    - compute gradient of training error w.r.t. $\tilde{\mathrm{s}}$
    - evaluate direct neighbor pointed to by gradient and compute its training error
    - if training error has decreased, jump to neighbor
    - if training error has not decreased, increase C_1 until gradient points to neighbor with smaller L_1-norm and smaller training error, and jump to that neighbor
  end while
end for

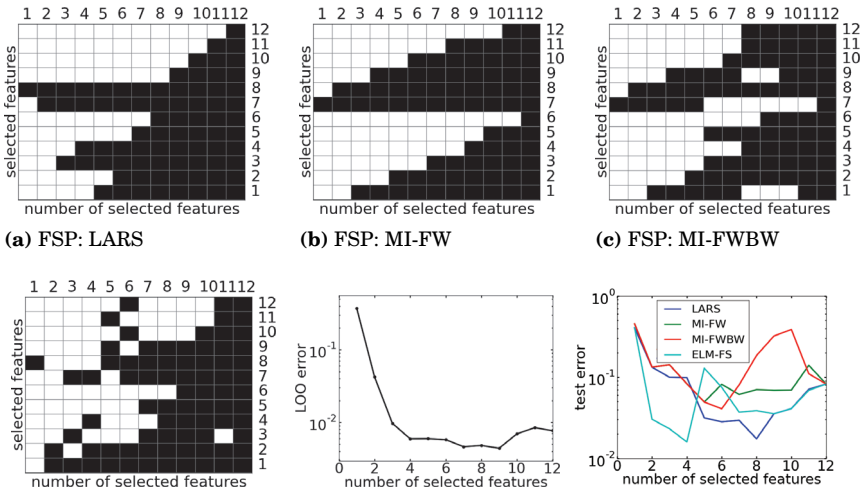
5.2.2 Feature selection path

During its execution, the ELM-FS algorithm (as described before and in detail in Publication III), keeps track of the optimal feature subsets it encounters for each feature subset size. Once finished, these results can be summarized in a plot depicting the Feature Selection Path (FSP). Apart from the optimal feature subset for each size, also the evolution of the feature subset can be seen, potentially giving insight into the problem at hand.

5.2.3 Sparsity-error trade-off curve

Besides the optimal feature selections encountered, the ELM-FS algorithm also keeps track of the corresponding estimated generalization error. These results can be summarized in the Sparsity-error trade-off curve (see Figure 5.1e for an example).

it gets stuck, increase the slope until it starts rolling again.



(a) FSP: LARS **(b)** FSP: MI-FW **(c)** FSP: MI-FWBW

(d) FSP: ELM-FS **(e)** SET curve: ELM-FS **(f)** test errors

Figure 5.1. Results on Santa Fe Laser Data set

Together, these plots can be used by the practitioner to make an informed decision about the optimal feature subset for the context.

5.2.4 Experiments

To evaluate the effectiveness of the ELM-FS algorithm, and to verify the soundness of the obtained variable selections, the ELM-FS algorithm is compared against several other methods for performing variable selection: (1) Least Angle Regression (LARS); (2) Forward Selection with Mutual Information criterion (MI-FW); (3) Forward-Backward Selection with Mutual Information criterion (MI-FWBW).

Once the feature selection paths for all methods are obtained, the test error is evaluated using an Optimally Pruned ELM (OP-ELM). This allows for verification that the SET curve indeed gives an indication of the optimal feature subset, and for comparison between the obtained variable selections of each method.

Data The data set used is again the Santa Fe Laser Data time series (Weigend and Gershenfeld, 1993), which consists of approximately 10000 samples, from which samples are obtained using a regressor size of 12.

Experimental parameters ELM-FS is performed using 100 repetitions. The 100 corresponding ELMs have between 1 and 100 randomly chosen neurons, drawn from a fixed set of 100 neurons. For more details see Publication III.

Comparison of feature selections The results of the experiment are summarized in Figure 5.1. It can be seen that in this experiment, especially for the smaller feature subsets, the ELM-FS is able to find better feature selections than the other methods. Presumably, this is due to its more thorough exploration of the sparser subsets, and the fact that ELM-FS allows for discontinuities in its feature selection path.

Comparison of computational times The computational efficiency of ELM-FS is comparable to MI-FW and MI-FWBW (see Table 2 of Publication III), and selected feature subsets are comparable or better in quality. Therefore, the ELM-FS provides an attractive alternative to existing feature selection methods.

5.3 Fast feature selection using a GPU-accelerated Delta Test

In Publication IV, a GPU-accelerated Delta Test criterion used as criterion in a parallelized genetic algorithm for variable selection. By using the GPU to accelerate the computation of the Delta Test, the main computational bottleneck of the algorithm is alleviated, and through GPU acceleration and parallelization variable selection with the Delta Test can efficiently be performed on large data sets, for which it would otherwise be prohibitively slow.

5.3.1 Parallelization of the Delta Test

Delta Test The Delta Test is a noise variance estimator which can be used to estimate, for a given data set $(x_i, y_i)_{i=1}^N$, the accuracy a non-linear model can possibly attain. Therefore, it can be used a criterion for evaluating the quality of different variable subsets for function approximation, and together with a search algorithm, be used for variable selection (Eirola, 2014; Sovilj, 2014). The Delta Test is defined as

$$\delta = \frac{1}{2N} \sum_{i=1}^{N} (y_i - y_{NN(i)})^2 \tag{5.4}$$

where y_i is the i^{th} sample in the output space, and $y_{NN(i)}$ is sample corresponding to the nearest neighbor of $\mathbf{x}_i$.

Computing the Delta Test From Equation 5.4, it can be seen that in order to compute the value of the Delta Test, for each sample $\mathbf{x}_i$, the nearest neighbor needs to be computed.

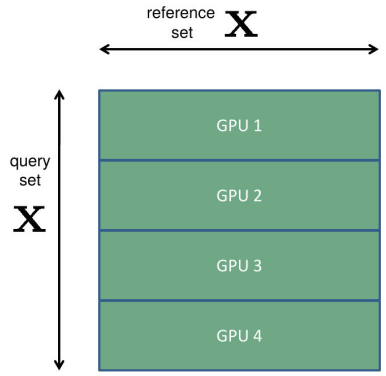


Figure 5.2. Division of nearest-neighbor computations in Multi-GPU-accelerated Delta Test

The approach used in Publication IV is the brute-force method for computing the nearest neighbors, which involves computing an $N \times N$ distance matrix. Once computed, for each $\mathbf{x}_i$, the index of the nearest neighbor can be determined from the distance matrix, and the Delta Test criterion can be computed. Since the approach involves computing an $N \times N$ distance matrix, for modern data sets this can be quite challenging, and strategies are desired for making the computation feasible.

Delta Test at scale The Delta Test is implemented on GPU using the excellent GPU-accelerated nearest-neighbor library by (Garcia et al., 2008, 2010), and for e.g. 17000 samples and with a 1000 variables, a 40-50$\times$ speedup can be obtained over using the CPU.

Although not exploited in Publication IV, the nearest-neighbor problem is embarrassingly parallel (i.e. the nearest neighbor for each point can be determined independently). Therefore, the Delta Test computation can be further accelerated by dividing the nearest-neighbor computations over multiple GPUs, and let each GPU determine the nearest neighbor for part of the data set (see Figure 5.2). Experiments show that for a variable selection problem with 100k samples and 274 dimensions, on a single machine with 5 GPUs, an additional speedup of roughly ~4$\times$ can be achieved.

Discussion The (multi-)GPU-acceleration of the Delta Test makes it a very attractive criterion to use as a filter approach for ELM, either in combination with a local search method like Forward-Backward search as encountered in Publication III, or in combination with genetic algorithm like in Publication IV.

5.4 Binary/Ternary ELM

Although in theory, ELM is a universal approximator, in practice, there are a limited number of samples available, and there is a risk of overfitting. Therefore, the functional approximation should use as limited number of neurons as possible, and the hidden layer should extract and retain as much information as possible from the input samples. The question then becomes, which neurons work well together to extract as much useful information as possible?

Publication V proposes two new ELM variants: Binary ELM, with a weight initialization scheme based on {0,1}-weights; and Ternary ELM, with a weight initialization scheme based on {-1,0,1}-weights. This weight initialization scheme results in features from very different subspaces and therefore, each neuron extracts more diverse information from the inputs than neurons with completely random features traditionally used in ELM. Experiments show that indeed ELMs with ternary weights generally achieve lower test error, and additionally are more robust to irrelevant and noisy variables. Since only the weight generation scheme is adapted, the computational time of the ELM is unaffected, and the improved accuracy, added robustness and the implicit variable selection of Binary ELM and Ternary ELM come for free.

5.4.1 Improved hidden layer weights

Traditionally, the hidden layer weights of the ELM are initialized randomly, with weights and biases drawn from a continuous probability distribution. For example, a uniform distribution on interval [-3, 3], or a Gaussian distribution with certain variance σ. These hidden layer weights, together with the transfer function and the data, result in particular activations of the hidden layer.

A typical transfer function (like sigmoid) takes the inner product of the weight and a sample, adds a bias, and transforms the result in a nonlinear way, i.e. it looks like $f\left(\langle \mathbf{w_i}, \mathbf{x} \rangle + b_i\right)$,where $\langle \mathbf{w_i}, \mathbf{x} \rangle$ is the inner product of weight $\mathbf{w}_i$ and $\mathbf{x}$ is the input vector. Since$\langle \mathbf{w_i}, \mathbf{x} \rangle = |\mathbf{w_i}||\mathbf{x}| \cos\theta$, it can be seen that the typical activation of f depends on:

1. the expected length of $\mathbf{w_i}$
2. the expected length of $\mathbf{x}$
3. the angles θ between the weights and the samples

5.4.1.1 Orthogonal weights?

An important factor affecting the diversity of the hidden neuron activations consists of the angles between the hidden layer weights and the samples. Therefore, the primary strategy that comes to mind for improving the diversity of the hidden neuron activations is to improve the diversity by taking weights that are mutually orthogonal (e.g. M d-dimensional basis vectors, randomly rotated in the d-dimensional space, where d is the dimension of the input space).

However, experiments suggested that this strategy does not significantly improve accuracy. Presumably, for the tested cases, the random weight scheme of ELM already covers the possible weight space pretty well (furthermore, randomly drawn zero-mean vectors are close to orthogonal in the first place).

5.4.1.2 Binary weight scheme

Another way to improve the diversity of the weights is by having each of them work in a different subspace (e.g. each weight vector has different subset of variables as input). This strategy turns out to significantly improve accuracy, at no extra computational cost.

In the binary weight scheme (see Algorithm 6, Figure 5.3 and Figure 5.4), binary weights are generated and added, starting from the sparsest subspace, until the desired amount of weights is reached. Weights within a subspace are added in random order to avoid bias towards particular variables. Once generated, the weights are normalized or adapted through Batch-Intrinsic Plasticity (BIP) pre-training (see Section 3.4.4 and Section 5.4.2) to ensure the neurons are activated in the right region (neither completely in the linear part, nor in the saturated part).

5.4.1.3 Ternary weight scheme

The ternary weight scheme (see Figure 5.3 and 5.4) is identical to the binary weight scheme, except that due to the sign of the weights there are more possible weights for each possible subspace, rather than a single one, allowing for richer weights.

5.4.2 Motivation for BIP pre-training

Since for given weight w and input x, the expected value of $|\mathrm{w}||\mathrm{x}|$ determines which part of the transfer function is activated most, the norm of the weights is important and affects the performance of ELM. Of course,

Algorithm 6 Binary weight scheme, with M the desired number of hidden neurons, n the dimension of the subspaces in which to generate weights, and d the number of inputs

1: *Generate ELM:*
2: $n = 1$;
3: **while** number of neurons $\leq M$ and $n \leq d$ **do**
4: - Generate the $\binom{d}{n}$ possible assignments of n ones to d positions
5: - Shuffle the order of the generated weights to avoid bias to certain inputs due to the scheme used to generate the $\binom{d}{n}$ assignments
6: - Add the generated weights (up to a maximum of M neurons)
7: - $n = n + 1$;
8: **end while**
9: - Normalize the norm of the weights, such that they are unit length.

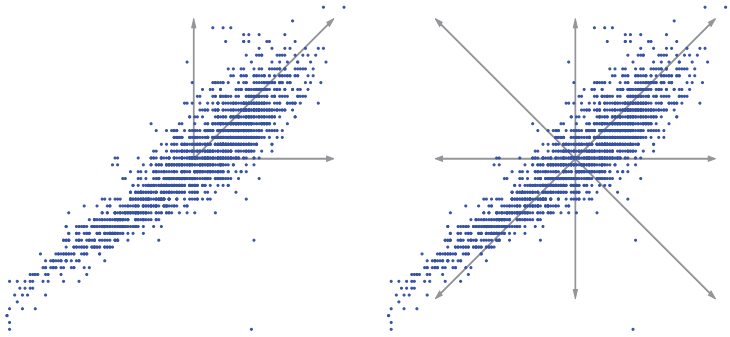
$$
\begin{array}{c|c}
 & \left[\begin{array}{ccccc}
\mathbf{1} & 0 & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & 0 & 0 \\
0 & 0 & \mathbf{1} & 0 & 0 \\
0 & 0 & 0 & \mathbf{1} & 0 \\
0 & 0 & 0 & 0 & \mathbf{1} \\
\hline
\mathbf{1} & \mathbf{1} & 0 & 0 & 0 \\
\mathbf{1} & 0 & \mathbf{1} & 0 & 0 \\
\mathbf{1} & 0 & 0 & \mathbf{1} & 0 \\
\mathbf{1} & 0 & 0 & 0 & \mathbf{1} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \mathbf{1} & \mathbf{1} \\
\hline
\multicolumn{5}{c}{etc.}
\end{array}\right] \\
\begin{array}{c} 1\,vars \\ \\ \\ \\ \\ \hline \\ \\ \\ \\ \\ \\ \hline 3\,vars \end{array} &
\end{array}
$$

(a) binary weight scheme

$$
\begin{array}{c|c}
 & \left[\begin{array}{cccc}
+\mathbf{1} & 0 & 0 & 0 \\
-\mathbf{1} & 0 & 0 & 0 \\
0 & +\mathbf{1} & 0 & 0 \\
0 & -\mathbf{1} & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots \\
\hline
+\mathbf{1} & +\mathbf{1} & 0 & 0 \\
+\mathbf{1} & -\mathbf{1} & 0 & 0 \\
-\mathbf{1} & +\mathbf{1} & 0 & 0 \\
-\mathbf{1} & -\mathbf{1} & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots \\
0 & 0 & -\mathbf{1} & -\mathbf{1} \\
\hline
\end{array}\right] \\
\begin{array}{c} 1\,vars \\ \\ \\ \\ \\ \hline \\ \\ \\ \\ \\ \\ \hline 3\,vars \end{array} &
\end{array}
$$

(b) ternary weight scheme

Figure 5.3. Illustration of the binary and ternary weight schemes. Note that weights are added starting from the sparsest subspace, and from each subspace they are added in random order to avoid bias towards particular variables.



(a) possible binary weights **(b)** possible ternary weights

Figure 5.4. Illustration of possible weights (*arrows*) for binary (*a*) and ternary (*b*) weight scheme, in a 2D subspace of normalized Abalone data (*blue dots*)

the weights could be normalized to be e.g. unit length, but the question remains what is the optimal length for the given data. Therefore, to ensure that the weights are properly scaled, the ELMs are pre-trained using Batch Intrinsic Plasticity (BIP) pre-training. In particular, the BIP(rand) variant (Neumann and Steil, 2011, 2013) is used, since it offers an attractive balance between computational time and accuracy.

An added advantage of using BIP pre-training is that when comparing ELMs with varying weight schemes, any differences in performance must come from the differences in the direction of the weights and are not a result of the different scaling of the weights.

Furthermore, since BIP pre-training adapts the neurons to operate in their non-linear regime, as many linear neurons are included as there are input variables. This ensures good performance of the ELM, even if the problem is completely linear.

5.4.3 Fast L2 regularization through SVD

With limited data, the capability of ELM to overfit the data increases with increasing number of neurons, especially if those neurons are optimized to be well-suited for the function approximation problem. Therefore, to avoid overfitting, Tikhonov regularization with an efficiently cross-validated regularization parameter is used.

Using the SVD decomposition of $\mathbf{H} = \mathbf{U}\mathbf{D}\mathbf{V}^T$, it is possible to obtain all needed information for computing the PRESS statistic without recomputing the pseudo-inverse for every λ:

$$
\begin{aligned}
\hat{\mathbf{Y}} &= \mathbf{H}\beta \\
&= \mathbf{H}(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{H}^T\mathbf{Y} \\
&= \mathbf{HV}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{DU}^T\mathbf{Y} \\
&= \mathbf{UDV}^T\mathbf{V}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{DU}^T\mathbf{Y} \\
&= \mathbf{UD}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{DU}^T\mathbf{Y} \\
&= \mathrm{HAT} \cdot \mathbf{Y}
\end{aligned}
$$

where $\mathbf{D}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{D}$ is a diagonal matrix with $\frac{d_{ii}^2}{d_{ii}^2+\lambda}$ as the i^{th} diagonal entry. Now

$$
\begin{aligned}
\mathrm{MSE}^{\text{TR-PRESS}} &= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - hat_{ii}}\right)^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - \mathbf{h}_{i\cdot}(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{h}_{i\cdot}^T}\right)^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - \mathbf{u}_{i\cdot}\left(\frac{d_{ii}^2}{d_{ii}^2+\lambda}\right)\mathbf{u}_{i\cdot}^T}\right)^2
\end{aligned}
$$

where $\mathbf{h}_{i\cdot}$ and $\mathbf{u}_{i\cdot}$ are the i^{th} row vectors of $\mathbf{H}$ and $\mathbf{U}$, respectively. Now, the Tikhonov-regularized PRESS and corresponding λ can be computed using Algorithm 7, where $\mathbf{A} \circ \mathbf{B}$ refers to the element-wise product of matrices $\mathbf{A}$ and $\mathbf{B}$ (Schur product). Due to the convex nature of criterion $\mathrm{MSE}^{\text{TR-PRESS}}$ with respect to regularization parameter λ, the Nelder-Mead procedure used for optimizing λ converges quickly in practice (Nelder and Mead, 1965; Lagarias et al., 1998). This efficient optimization of the regularization parameter for ELM, by incorporating it in the SVD decomposition first appeared (in slightly different form) in (Miche et al., 2011).

5.4.4 Experiments

In Publication V, for evaluating the performance of the gaussian, binary and ternary weight schemes, their resulting performance in terms of accuracy is compared on various regression tasks. Since the weight range determines the typical activation of the transfer function (remember $\langle \mathbf{w_i}, \mathbf{x} \rangle = |\mathbf{w_i}||\mathbf{x}| \cos\theta$), the ELMs are pre-trained using Batch Intrinsic Plasticity pre-training. Any performance difference between weight schemes will be a result of the different directions of the weights. Furthermore, since BIP pre-training adapts the neurons to operate in their non-linear regime, as many linear neurons are included as there are input variables. This ensures good performance of the ELM, even if the problem is completely

Algorithm 7 Tikhonov-regularized PRESS. In practice, the **while** part of this algorithm (convergence for λ) is solved using by a Nelder-Mead approach (Nelder and Mead, 1965) (Publication V)).

1: Decompose $\mathbf{H}$ by SVD: $\mathbf{H} = \mathbf{U}\mathbf{D}\mathbf{V}^T$
2: Precompute $\mathbf{B} = \mathbf{U}^T\mathbf{y}$
3: **while** no convergence on λ achieved **do**
4: - Precompute $\mathbf{C} = \mathbf{U} \circ \begin{pmatrix} \frac{d_{11}^2}{d_{11}^2+\lambda} & \cdots & \frac{d_{11}^2}{d_{11}^2+\lambda} \\ \vdots & \ddots & \vdots \\ \frac{d_{NN}^2}{d_{NN}^2+\lambda} & \cdots & \frac{d_{NN}^2}{d_{NN}^2+\lambda} \end{pmatrix}$
5: - Compute $\hat{\mathbf{y}} = \mathbf{C}\mathbf{B}$, the vector containing all $\hat{y}_i$
6: - Compute $\mathbf{d} = \text{diag}\left(\mathbf{C}\mathbf{U}^T\right)$, the diagonal of the HAT matrix, by taking the row-wise dot-product of $\mathbf{C}$ and $\mathbf{U}$
7: - Compute $\varepsilon = \frac{\mathbf{y}-\hat{\mathbf{y}}}{\mathbf{1}-\mathbf{d}}$, the leave-one-out errors
8: - Compute $\text{MSE}^{\text{TR-PRESS}} = \frac{1}{N}\sum_{i=1}^{N}\varepsilon_i^2$
9: **end while**
10: Keep the best $\text{MSE}^{\text{TR-PRESS}}$ and the associated λ value

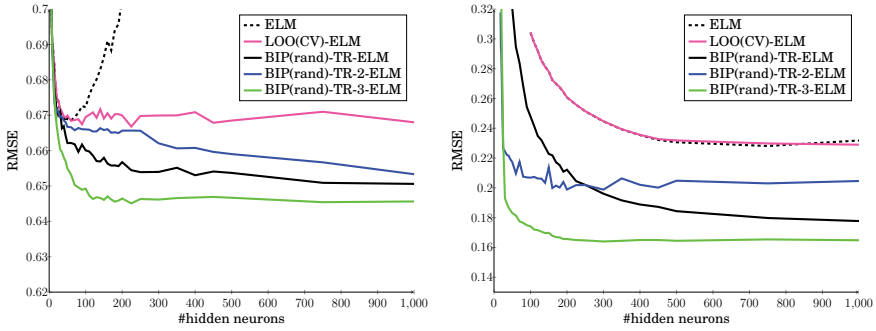
linear. Finally, to prevent overfitting, the models incorporate L2 regularization with efficiently optimized regularization parameter (as described in Section 5.4.3). Therefore, in summary, the models that are compared are the BIP(rand)-TR-ELM; the BIP(rand)-TR-2-ELM and the BIP(rand)-TR-3-ELM.

Data The data sets used for the experiments are the Abalone (8 input variables, 4177 samples) and ComputerActivity (12 input variables, 8192 samples) data sets from the UCI repository (Asuncion and Newman, 2007). Roughly half of the samples is used for training, and the remaining half is used for testing.

Relative performance of weight schemes In this experiment, the relative performance of the weight schemes is compared for varying number of hidden neurons. As mentioned, the ELMs are pre-trained through BIP, and use L2 regularization with efficiently optimized regularization parameter. As further baseline, a standard ELM and an ELM which has its number of neurons cross-validated are included as well. The results of this experiment are summarized in Figure 5.5.

There, it can be seen that for increasing number of neurons, the standard ELM starts to overfit at some point, resulting in an increase in the RMSE on the test set. Performing leave-one-out cross-validation to limit the number of used hidden neurons prevents this overfitting. Finally, the

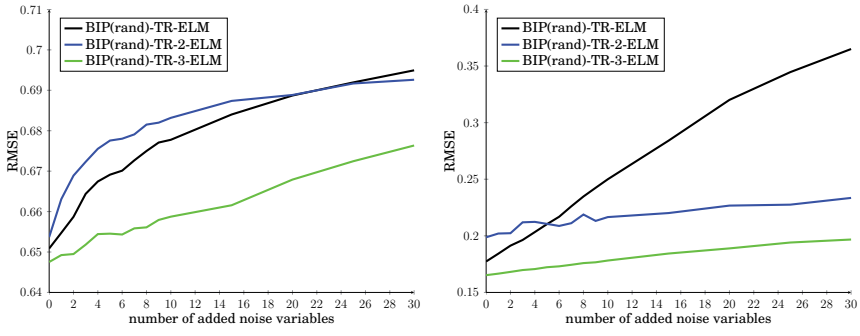
proposed methods generally achieve much better RMSE than the basic ELM variants and generally, ternary weights outperform weights drawn from a Gaussian distribution, while binary weights perform worse than ternary and Gaussian weights for large number of neurons.



(a) Abalone **(b)** ComputerActivity

Figure 5.5. number of neurons vs. average achieved test RMSE for ELM (*black, dashed*), LOO(CV)-ELM (*purple*), BIP(rand)-TR-ELM with Gaussian (*black*), binary (*blue*), ternary (*green*) weight scheme (Publication V).

Robustness against irrelevant variables In this experiment, the robustness of the different weight schemes against irrelevant variables is investigated by measuring the effect of up to 30 added noise variables on the RMSE. The results are summarized in Figure 5.5 and Table 5.1, where it can be seen that the proposed weight schemes are more robust against irrelevant variables. The difference is especially large for the ComputerActivity Data set.



(a) Abalone **(b)** ComputerActivity

Figure 5.6. Effect of adding irrelevant extra variables on RMSE for BIP(rand)-TR-ELM with 1000 hidden neurons and with Gaussian (*black*), binary (*blue*), ternary (*green*) weight scheme (Publication V).

	Ab			Co		
	gaussian	binary	ternary	gaussian	binary	ternary
RMSE with original variables	0.6497	0.6544	0.6438	0.1746	0.1785	0.1639
RMSE with 30 added irr. vars	0.6982	0.6932	0.6788	0.3221	0.2106	0.1904
RMSE loss	0.0486	**0.0388**	**0.0339**	0.1475	**0.0321**	**0.0265**

Table 5.1. Effect of adding irrelevant extra variables on RMSE for BIP(rand)-TR-ELM with 1000 hidden neurons and with gaussian, binary, and ternary weight scheme (Publication V).

Implicit variable selection Finally, to get more insight into why the weight schemes perform the way they do, the BIP(rand)-TR-ELM, BIP(rand)-TR-2-ELM and the BIP(rand)-TR-3-ELM are trained on the ComputerActivity data set, where 5 irrelevant variables (taken from the DeltaElevators UCI data) and 5 noise variables have been added.

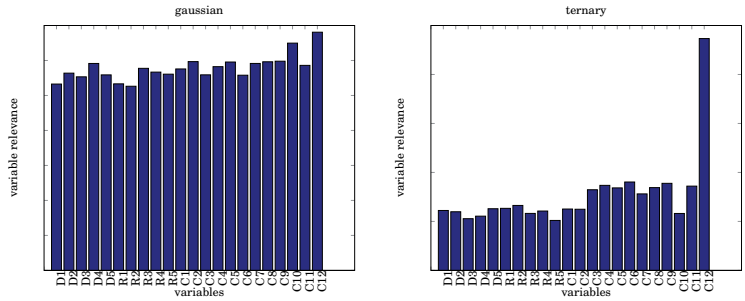
After training, the relevance of each input variable is quantified as

$$\mathbf{relevance} = \sum_{i=1}^{M} |\beta_i \times \mathbf{w}_i|,$$

where M is the number of hidden neurons; β_i is the output weight; $\mathbf{w}_i$ is the input weight corresponding to neuron i, and $\mathbf{relevance}$ is the d-dimensional vector containing a measure of relevance for each of the d input variables. If a variable j has a large value of $\mathbf{relevance}_j$, compared to other variables, this can be interpreted as that variable being implicitly selected by the ELM (i.e. the ELM favors neurons that extract information from that variable).

The results are summarized in Figure 5.7, and suggest qualitatively different behaviour of the ELMs with the different weight schemes. While the BIP(rand)-TR-ELM does not favor any neurons that employ a particular input variable, the BIP(rand)-TR-3-ELM favors neurons that employ a specific input variable. Similar results hold for BIP(rand)-TR-2-ELM.

These results suggests that the improved performance and robustness of the binary and ternary weight scheme might come from implicit variable selection, and that through the modified weight schemes, they are able to focus on those variables that are important to the problem, while ignoring the variables that are not.



(a) Gaussian weight scheme **(b)** Ternary weight scheme

Figure 5.7. Relevance assigned by the weight schemes to different input variables, as measured by $\sum_{i=1}^{M} |\beta_i \times \mathbf{w}_i|$ (Publication V).

Discussion Two new weight initialization schemes have been proposed and robust ELM variants using these weight schemes are introduced and evaluated: the BIP(rand)-TR-2-ELM and BIP(rand)-TR-3-ELM.

The motivation behind these schemes is that weights picked in this way will be from very different subspaces, and therefore improve the diversity of the neurons in the hidden layer.

Experiments show that Ternary ELM generally achieves lower test error and that both the binary and ternary weight schemes improve robustness of the ELM against irrelevant and noisy variables, which might be due to the schemes being able to perform implicit variable selection. Since only the weight generation scheme is changed, the computational time of ELM remains unchanged compared to ELMs with traditional random weights. Therefore, the better performance, added robustness and implicit variable selection in Binary ELM and Ternary ELM come for free.

Although this work only investigates the robustness of the weight schemes, an additional advantage of the proposed weight schemes is that they result in sparse weight matrices. Especially for large ELMs, this can result in significantly reduced memory requirements, since the weight matrices can be saved as sparse matrices with binary or ternary entries[3]. Furthermore, algorithms designed for sparse matrix multiplication might be used to speed up the multiplication of the inputs and the hidden layer weights. This could potentially provide a further way to speed up existing MapReduce schemes for accelerating the hidden layer computations (Catanzaro et al., 2008; He et al., 2011, 2013).

[3]Although the weights of each neuron are normalized, all weights of a neuron are scaled with the same scalar, which can be incorporated in e.g. the slope of the sigmoid transfer function.

6. Trade-offs in Extreme Learning Machines

> *"There are all kinds of interesting questions that come from a knowledge of science, which only adds to the excitement and mystery and awe of a flower. It only adds. I don't understand how it subtracts."*
>
> – Richard P. Feynman

In the training of neural networks, there often exists a trade-off between the time spent optimizing the model under investigation, and its final performance. Ideally, an optimization algorithm finds the model that has best test accuracy from the hypothesis space as fast as possible, and this model is efficient to evaluate at test time as well. However, in practice, there exists a trade-off between training time, testing time and testing accuracy, and the optimal trade-off depends on the user's requirements.

This chapter gives an overview of some of those trade-offs within the context of ELMs and highlights the results from Publication VI, which introduces the Compressive ELM and forms an initial investigation into these trade-offs within Extreme Learning Machines.

Whereas the other contributions are mostly aimed at directly improving the accuracy of the ELM-based methods, either by ensembling them (Publication I, Publication II), by obtaining better variable selections (Publication III, Publication IV), or by improved weight initialization schemes (Publication V), the Compressive ELM takes a contrary approach.

Instead of directly improving the accuracy, the Compressive ELM focuses on improving the computational time by providing a time-accuracy trade-off and training the model in a reduced space, while trying to retain accuracy as much as possible. Experiments indicate that potentially more time can be saved than accuracy lost and therefore the compressive training mechanism may provide an avenue towards obtaining more accurate models in less time.

6.1 Trade-offs between computational time and accuracy

When choosing a model for solving a machine learning problem, which model is most suitable depends a lot on the context and the requirements of the application. For example, it might be the case that the model is trained on a continuous stream of data, and therefore has some restrictions on the training time. On the other hand, the computational time in the testing phase might be restricted, like in a setting where the model is used as the controller for an aircraft or a similar setting that requires fast predictions. Alternatively, the context in which the model is applied might not have any strong constraints on the computational time and, above all, accuracy or interpretability could be considered most important regardless of the computational time.

6.1.1 Time-accuracy curves

This chapter focuses on time-accuracy trade-offs in Extreme Learning Machines, and on trade-offs between training time and accuracy in particular, which can be affected in two ways:

- by **improving the accuracy** through spending more time optimizing the model,

- or vice-versa, by **reducing the computational time** of the model, without sacrificing accuracy too much.

Each type of model has its own ways of balancing computational time and accuracy, and has an associated training time-accuracy curve that expresses the efficiency of the model in achieving a certain accuracy (the closer the curve is to the bottom left, the better). Thus, given a collection of models, the question becomes: which model produces the best accuracy the fastest?

6.1.2 Examples from Extreme Learning Machines

In order to illustrate what time-accuracy trade-offs exist within Extreme Learning Machines, this section presents time-accuracy trade-offs of several Extreme Learning Machine variants.

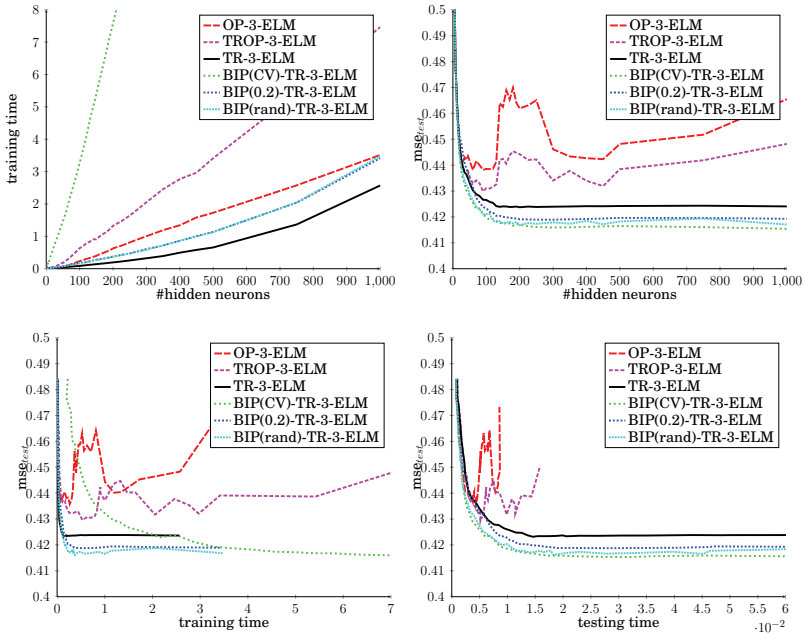


Figure 6.1. Results for various ELM variants on Abalone UCI data set (Publication V).

Extreme Learning Machine variants The following variants of Extreme Learning Machine are compared in terms of their training time, testing time, and obtained accuracy on the Abalone UCI data set (Asuncion and Newman, 2007). For all of the variants, the ternary weight scheme is used, because of the benefits shown in Publication V, and Section 5.4. The Tikhonov-regularized variants all use efficient optimization of regularization parameter λ, using the SVD approach to computing $\mathbf{H}^{\dagger}$ (see Section 5.4.3).

OP-ELM The Optimally Pruned ELM (Miche et al., 2010), with neurons ranked by relevance, and then pruned based on the leave-one-out error.

TROP-ELM The Tikhonov-regularized OP-ELM (Miche et al., 2011).

TR-ELM The Tikhonov-regularized ELM (Deng et al., 2009).

BIP(CV)/BIP(0.2)/BIP(rand) TR-ELM The Tikhonov-regularized ELM pre-trained using Batch Intrinsic Plasticity mechanism (Neumann and Steil, 2011, 2013; Neumann, 2013), adapting the hidden layer weights and biases, such that they retain as much information as possible. The BIP parameter is either fixed, randomized, or cross-validated over 20 possible values.

Most desirable model depends on requirements The results are summarized in Figure 6.1, and show that it depends on the user's criteria which model is most suitable for that context.

Training time most important If it is most important that the model can be trained fast, then it can be argued that the BIP(rand)-TR-3-ELM offers the best trade-off. It does take slightly longer to train than the TR-3-ELM, however, for that modest overhead the test accuracy is generally improved.

Test error most important If accuracy is all that matters, then the results suggest it might be worth it to cross-validate the BIP parameter, instead of setting it randomly per-neuron. Although the training time for BIP(CV)-TR-3-ELM is many times higher due to the cross-validation of the BIP parameter, it generally results in the most accurate model.

Testing time most important If the speed of the model at test time is most important, then, surprisingly, the results suggest that the BIP(rand)-TR-3-ELM is the most suitable model. This result is unexpected, since a model that has its irrelevant neurons pruned (like OP-ELM and TROP-ELM) is generally faster at test time. However, for this context, the results reveal that, even though the OP-ELM and TROP-ELM are faster, they tend to slightly overfit while pruning the neurons, resulting in slightly worse test accuracy.

From Figure 6.1, it can be seen that because of this, the TR-3-ELM variants are more attractive when it comes to testing time (i.e. for a given testing time, they are always able to provide the better accuracy).

This surprising result shows the importance of analyzing ELM algorithms in terms of their time-accuracy trade-off. Furthermore, this time-accuracy trade-off analysis suggests further research directions into the prevention of overfitting in model structure selection (Reunanen, 2003).

An initial work along these lines is (Wang et al., 2014), which provides a variant of OP-ELM that computes an approximate ranking of the neurons, rather than an exact ranking, and is shown to achieve better accuracy. Presumably, this is because the approximate ranking prevents the model structure selection from overfitting.

Since TR-3-ELM offers attractive trade-offs between speed and accuracy, this model is used for the Compressive Extreme Learning Machine, which will be discussed next.

6.2 Compressive ELM

In the previous section on time-accuracy trade-offs, two possible strategies have been discussed that can affect this trade-off: (1) improving the accuracy of the models, and (2) reducing the computational time of the model. In terms of training time-accuracy plots, this would be "pushing the curve down" and "pushing the curve to the left", respectively.

Whereas the other contributions discussed in this thesis mainly focus on improving the accuracy of the models by ensembling them (Publication I, Publication II), by obtaining better variable selections (Publication III, Publication IV), or by improved weight initialization schemes (Publication V), the Compressive ELM focuses on reducing computational time by performing the training in a reduced space, while retaining accuracy as much as possible.

6.2.1 Low-distortion embeddings

To achieve this, the dimensionality of the hidden layer output matrix is reduced by creating a low-distortion embedding of it in a lower-dimensional space through Johnson-Lindenstrauss-like embeddings (Johnson and Lindenstrauss, 1984; Achlioptas, 2003; Matoušek, 2008), which approximately preserve the distances between the points and retain the relevant structure as much as possible. These embeddings occur in approximate distance-based machine learning algorithms like approximate nearest-neighbors (Indyk and Motwani, 1998), and are extensively used in the field of Randomized numerical linear algebra (Martinsson, 2009).

6.2.2 Randomized numerical linear algebra

Part of many algorithms in randomized numerical linear algebra is the embedding (or sketching) of the data into a lower dimension. In comparison to distance-based methods though, in linear algebra, the requirement for preserving the distances is not as strict, and as long as the distances are roughly preserved (within some factor) it is useful (Martinsson, 2009).

One aspect of linear algebra in which low-distortion embeddings can be used is in approximate matrix decomposition. Given a matrix, an approximate matrix decomposition can be achieved by first embedding the rows of the matrix into a lower-dimensional space (through one of many available low-distortion Johnson-Lindenstrauss-like embeddings), solving the

decomposition, and then projecting back to the full space. If such an embedding (or sketch) is accurate, then this allows for solving the problem with high accuracy in reduced time. An example of such an algorithm is the approximate SVD.

Approximate SVD The algorithm for approximate SVD is summarized in Algorithm 8. More background on the algorithm can be found in (Halko et al., 2011).

Algorithm 8 Approximate SVD (Halko et al., 2011) (Publication V).

Given an $m \times n$ matrix $\mathbf{A}$, compute k-term approximate SVD $\mathbf{A} \approx \mathbf{U}\mathbf{D}\mathbf{V}^T$as follows:

1: - Form the $n \times (k+p)$ random matrix $\mathbf{\Omega}$. (where p is small oversampling parameter)
2: - Form the $m \times (k+p)$ sampling matrix $\mathbf{Y} = \mathbf{A}\mathbf{\Omega}$. ("sketch" it by applying $\mathbf{\Omega}$)
3: - Form the $m \times (k+p)$ orthonormal matrix $\mathbf{Q}$, such that range$(\mathbf{Q}) =$ range$(\mathbf{Y})$.
4: - Compute $\mathbf{B} = \mathbf{Q}^*\mathbf{A}$.
5: - Form the SVD of $\mathbf{B}$ so that $\mathbf{B} = \hat{\mathbf{U}}\mathbf{D}\mathbf{V}^T$
6: - Compute the matrix $\mathbf{U} = \mathbf{Q}\hat{\mathbf{U}}$

Application to ELM Through the approximate SVD, the time it takes to train the ELM can be reduced. Furthermore, the efficient L2 regularization from Section 5.4.3 can be easily integrated in it as well. The main question now is, whether it is actually possible to obtain more accurate models in less time.

Before giving an overview of the experiments investigating this, the next section gives a short overview of fast sketching algorithms that can be used as part of the approximate SVD algorithm.

6.2.3 Faster Sketching

Typically, the bottleneck in Algorithm 8 is the time it takes to sketch the matrix. Rather than using a class of random matrices of Gaussian variables for sketching A, one can also use random matrices that are sparse or structured in some way (Achlioptas, 2003; Matoušek, 2008), and for which the matrix-vector product can be computed more efficiently. Furthermore, (Ailon and Chazelle, 2006) introduced the Fast Johnson-Lindenstrauss Transform (FJLT), which uses a class of random matrices that permit ap-

plication to vectors from an $n \times n$ matrix to a vector in $\mathcal{O}(n \log(n))$, rather than the usual $\mathcal{O}(n^2)$. Besides this obvious speedup, this class of matrices is also more successful in creating a low-distortion embedding when applied to a sparse matrix. These transforms consist of the application of three easy-to-compute matrices

$$\left(\mathbf{P} \right)_{k \times n} \left(\mathbf{W} \right)_{n \times n} \left(\mathbf{D} \right)_{n \times n}$$

where $\mathbf{P}$, $\mathbf{W}$, and $\mathbf{D}$ vary depending on the exact scheme. Generally, $\mathbf{D}$ is a diagonal matrix with random Rademacher variables $\{-1, +1\}$ on the diagonal. In this work, the following transforms are considered for faster sketching:

- **Fast Johnson Lindenstrauss Transform (FJLT)**, introduced in (Ailon and Chazelle, 2006) for which $\mathbf{P}$ is a sparse matrix of random Gaussian variables, and $\mathbf{W}$ encodes the Discrete Walsh-Hadamard Transform.

- **Subsampled Randomized Hadamard Transform (SRHT)**, for which $\mathbf{P}$ is a matrix selecting k random columns from $\mathbf{W}$, and $\mathbf{W}$ encodes the Discrete Walsh-Hadamard Transform.

Both sketching methods were implemented for the Compressive ELM by adapting the excellent Blendenpik library (Avron et al., 2010).

6.2.4 Experiments

The experiments of Publication V investigate the trade-off between computational time (both training and test), and the accuracy of the Compressive ELM in relation to the dimensionality of the space into which the problem is reduced, using the sketch. For sketching, Compressive TR-3-ELMs with a Gaussian, FJLT, and SRHT sketching scheme are considered, and compared with the standard TR-3-ELM.

Data The experiments are performed using the CaliforniaHousing data set (Asuncion and Newman, 2007), and the data is divided randomly into 8000 random samples for training and the remaining 12640 samples for testing.

Experimental parameters The number of hidden neurons in each model is varied between 2 and 1000, and parameter $k = [50, 100, 200, 400, 600]$.

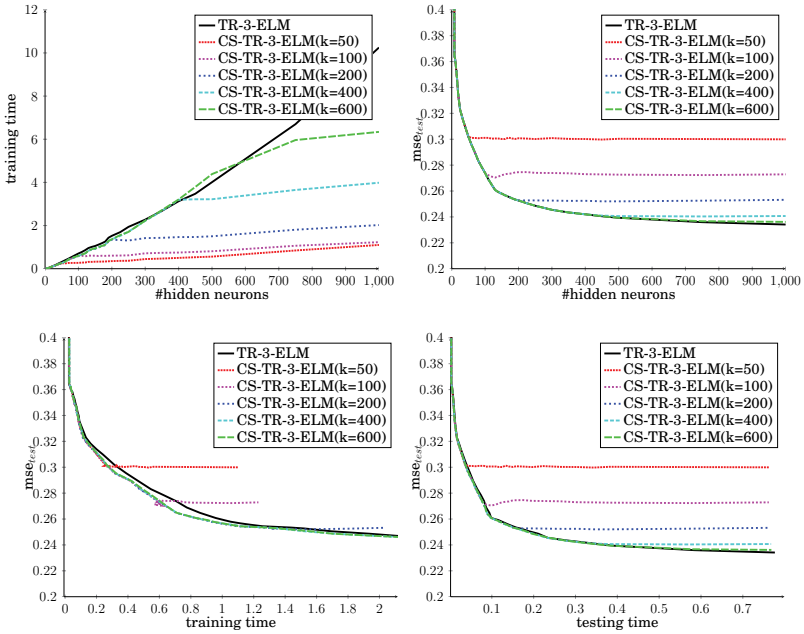


Figure 6.2. Results for Compressive ELMs using FJLT sketching with varying k on CaliforniaHousing UCI data set (Publication V).

Experiments are repeated with 200 random realizations of the training and test set, and average results over those 200 runs are reported.

Effect of embedding dimension Figure 6.2 shows the time-accuracy trade-offs achieved by the various methods, and shows the effect of the embedding dimension. Although only the results of FJLT sketching are presented here, similar results hold for the other sketching methods. It can be seen that

- setting k lower than the number of neurons results in faster training times (which makes sense since the problem solved is smaller).

- as long as parameter k is chosen large enough, the method is not losing efficiency (i.e. there is no model that achieves better error in the same computational time), and it is potentially gaining efficiency (as shown by the bottom-left plot of Figure 6.2.

Effect of embedding scheme Finally, the experiments showed that sketches with Gaussian matrices are generally the fastest, and for the tested problem sizes, the SRHT is slightly faster than the FJLT.

Discussion Surprisingly, the experiments did not show substantial differences in terms of computational time for the different embedding schemes. Therefore, for the datasets tested, it seems that although FJLT permits faster matrix multiplications, no advantage could be taken of it in the tested problems. More research is required to gain more insight into this behaviour, and to understand in what contexts the FJLT can effectively be exploited.

Furthermore, the results indicate that although the Compressive ELM provides an effective trade-off between time and accuracy, in this case, little compression could be obtained for the information in the hidden layer: as soon as k is set lower than the number of neurons, the accuracy decreases accordingly. This challenge to significantly compress the information in the hidden layer might be due to the quality of the features used in the Tikhonov-regularized Ternary Compressive ELM: they might result in a full-rank matrix that has no redundancies. However, more research is needed to better understand in what architectures and applications the Compressive ELM can effectively compress the randomly extracted features.

In summary, the Compressive ELM provides a way for trading off computational time and accuracy, by performing the training in a reduced space, using low-distortion embeddings and approximate matrix decompositions based on them. Experiments indicate that through this mechanism, potentially more time can be saved than accuracy lost and therefore the compressive training mechanism may provide a way to obtain more accurate models in less time.

Finally, developing low-distortion embeddings and related theoretical results is currently a very active field of research, and new developments in this area can be readily integrated to improve the performance of Compressive ELM.

7. Conclusions and Discussion

7.1 Contributions

The thesis develops several ensembling strategies based on ELM that can be applied in nonstationary environments and to large-scale learning problems. Due to the fine-grained structure of the ensemble models, they are very flexible, and can be evaluated in a parallel fashion. The individual models can be built and evaluated efficiently by performing the training and model structure selection on GPUs. Finally, the (adaptive) combination of diverse individual models results in a more accurate model. The models themselves can be relatively simple, while due to ensembling the overall model is still accurate. The results suggest this to be an accurate, yet flexible approach that can be used for analyzing large-scale potentially nonstationary streams of data.

Furthermore, several very different variable selection strategies have been explored. Firstly, in the ELM-FS, the use of the ELM architecture for variable selection, through relaxation of the variable selection problem is investigated. Besides providing a good subset of variables, the presented approach determines for each subset size, which variable subset would be best, and how the generalization error is expected to change depending on the number of variables selected. This provides insight into the problem, and allows for an informed decision on the variable subset that is best for the current context. Secondly, a filter method is presented for variable selection, which allows for variable selection in large-scale problems through the use of (multi-)GPU-acceleration of the Delta Test criterion, used in a parallelized genetic algorithm. Finally, new binary and ternary random weight schemes for ELM are developed, which result in more accurate and compact models. Experiments suggest that the

changed weight schemes make the ELM more robust to noisy and irrelevant variables, and are therefore a promising target for future research.

Finally, an approach was presented for reducing the computational time needed for training the ELM by embedding the random feature expansions in a lower-dimensional space. This allows for a flexible trade-off between accuracy and speed of the ELM, and could potentially reduce redundancy in the hidden neurons, resulting in more effective models. Experiments suggest that this approach may provide a path towards obtaining more accurate models in less time.

Overall, the collection of proposed methods provides an efficient, accurate and flexible framework for solving large-scale supervised learning problems. Several distinct strategies are explored for obtaining faster and more accurate models that are particularly suited for handling modern large-scale data sets. The developed methods are not limited to the particular types of ELMs and contexts in which they have been tested, and they may be readily combined, adapted and integrated for application in different contexts and models.

7.2 Future directions

Of course research is a continuing process, and every new development and result brings new questions. To conclude, this section gives a short overview of some of those possible future research directions.

Better training and regularization strategies Several results from the thesis suggest the importance of proper regularization for obtaining an accurate model and preventing overfitting. Furthermore, recent results in deep learning (Ba and Caruana, 2014), suggest that the success of deep neural networks may be due to the way they are trained, rather than just their architecture: i.e. it is possible to train a shallow mimic network based on an already trained deep network, which attains better accuracy than when a shallow network is trained directly. Perhaps what is missing for shallow networks, in order to obtain as good or similar performance as deep networks, is the right algorithm?

Therefore, an important line of research is exploring alternative training and regularization strategies in ELM-based architectures. What is the best strategy in training and performing model structure selection, such that the model obtains high accuracy and does not suffer from overfitting?

Improved data-agnostic random features The results from the Binary and Ternary ELM suggest that improved data-agnostic random features can be obtained by using weight initialization schemes other than the ones typically used in hidden layer initialization. Why exactly does one weight scheme work better than another, and can insights into this inform on even better weight schemes?

Overall then, aside from the question “what is the best accuracy a model can achieve?”, in my opinion the more interesting question is “what is the most effective way to achieve this accuracy?”. What routes exist towards obtaining optimal performance, and what effective shortcuts exist along the way for getting there faster?

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Nowadays, due to advances in technology, the size and dimensionality of data sets used in machine learning have grown very large and continue to grow by the day. For this reason, it is important to have efficient computational methods and algorithms that can be applied to large data sets, such that it is still possible to complete the machine learning task in reasonable time.

This dissertation introduces several machine learning methods based on Extreme Learning Machines (ELMs), meant to deal with these challenges. It focuses on developing efficient, yet accurate and flexible methods. These contributions take three main directions. Firstly, ensemble approaches based on ELM, that adapt to context and can scale to large data. Secondly, ELM-based variable selection approaches, that result in more accurate and efficient models. Finally, training algorithms for ELM that allow for a flexible trade-off between accuracy and computational time.

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