Table of Contents

Table of contents i

Table of figures iv

Table of tables xi

Foreword xii

Motivation and Abstract xvi

Nomenclature xix

1 Different tools for Modeling 1

1.1 Curve Fit 2

1.2 Splines 11

1.2.1 Ordinary Splines 12

1.2.1.1 Algorithm 12

1.2.1.2 Results and Limitations 14

1.2.2 B-Splines 15

1.2.2.1 Algorithm 15

1.2.2.2 Results and Limitations 16

1.3 Neural Networks 19

1.3.1 Backpropagation Neural Networks 19

1.3.1.1 Structure and Algorithm of a Backpropagation Neural Network 19

1.3.1.2 Training of a Backpropagation Neural Network 24

1.3.1.3 Pros and Cons of Backpropagation Neural Nets 28

1.3.2 Probabilistic Neural Network 29

1.3.2.1 The Bayes Strategy for Pattern Classification 29

1.3.2.2 Probabilistic Neural Network 35

1.3.3 Why Probabilistic Neural Networks and not Backpropagation Neural Networks? 39

1.4 Chapter Summary 41

2 General Regression Neural Network (GRNN) 42

2.1 Algorithm 43

2.2 How to choose σ 47

2.2.1 The Holdout Method 51

2.2.2 The Wiggle-Method 54

2.3 Extreme points 62

2.4 Unequally spaced data 64

2.5 Multi-Dimensions 69

2.6 Measurement Errors 71

2.7 Extrapolation 73

2.8 Underlying function 75

2.9 Chapter Summary 81

3 Application of GRNN to a Heat Exchanger 83

3.1 The heat exchanger 84

3.2 Training Samples for the Prediction 89

3.3 Influence of Simple model on Prediction 91

3.4 Multi-Dimensions 114

3.5 Influence of Measurement errors 126

3.6 Chapter Summary 139

4 Conclusion and Recommendations 141

References 146

Appendix, GRNN

149

Table of figures

Fig. 1.1-1 Oscillating mass on Spring 3

Fig. 1.1-2 Curve Fit for Polynomial and physical relationship 5

Fig. 1.1-3 Extrapolating abilities of polynomial and mechanistic relationship 8

Fig. 1.1-4 Using different functions for curve fit, for biased data 10

Fig. 1.2-1 Result for a ordinary Spline Function 12

Fig. 1.2-2 Comparison of ordinary Spline for slightly noisy data compared to non-noisy data 14

Fig. 1.2-3 general B-spline 15

Fig. 1.2-4 B-Spline with not enough sections 17

Fig. 1.2-5 B-Spline including different additional information and not 18

Fig. 1.3-1 Fig organization of neural network 21

Fig. 1.3-2 Sigmoid function and Threshold function 23

Fig. 1.3-3 Backpropagation neural network, nomenclature used for learning description 25

Fig. 1.3-4 Block Diagram for Backpropagation Learning Algorithm [Zurada] 27

Fig. 1.3-5 Decision surface between states of nature A and B 31

Fig. 1.3-6 Block diagram of a Probabilistic Neural Network 36

Fig. 1.3-7 Process in a Pattern Unit 38

Fig. 1.3-8 Distance between the training sample and the point of prediction 39

Fig. 2.1-1 GRNN with individual terms contributing to prediction, s=0.1 45

Fig. 2.1-2 GRNN built up in a way such that it can be used as a parallel Neural Network 46

Fig. 2.2-1 GRNN Prediction with extreme wiggles, including the individual signals, σ=0.027 48

Fig. 2.2-2 Prediction with GRNN for a big smoothness parameter, σ =1.0 50

Fig. 2.2-3 Result from Holdout Method 53

Fig. 2.2-4 Using s as suggested by the Holdout Method and other s to compare 54

Fig. 2.2-5 Wiggle-method 56

Fig. 2.2-6 Selection of σ 57

Fig. 2.2-7 Prediction and Slope of Prediction for a very smooth curve, σ =0.1 59

Fig. 2.2-8 Prediciton and Slope of Prediction for a curve with many wiggles, σ=0.027 60

Fig. 2.3-1 GRNN with Problem at extreme points 61

Fig. 2.4-1 GRNN with problems having unequally spaced training samples, two inflections were allowed 64

Fig. 2.4-2 GRNN with problems having unequally spaced training samples, four inflections were allowed 65

Fig. 2.4-3 Nonparametric Regression 66

Fig. 2.5-1 A way to circumvent the influence of multi-dimensionality for independence of the inputs 69

Fig. 2.6-1 GRNN prediction of data including measurement errors, 2 inflection points allowed 71

Fig. 2.6-2 GRNN prediction of data including measurement errors, 4 inflection points allowed 71

Fig. 2.7-1 Extrapolation ability of GRNN 72

Fig. 2.8-1 Different prediction methods, using only training samples and using an underlying function in addition to training samples 75

Fig. 2.8-2 Influence of an underlying function on the extreme values 77

Fig. 2.8-3 Influence of an underlying function on the effects of unequally spaced data, two inflection were allowed 78

Fig. 2.8-4 Influence of an underlying function on the effects of unequally spaced data, four inflections were allowed 79

Fig. 3.1-1 The Heat exchanger 82

Fig. 3.3-1 Efectiveness versus mass flow rate using 81 samples, equally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=12.5m/s 92

Fig. 3.3-2 Effectiveness versus mass flow rate using 81 samples equally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=25m/s 93

Fig. 3.3-3 Effectiveness versus mass flow rate using 500 samples unequally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=12.5m/s 95

Fig. 3.3-4 Effectiveness versus mass flow rate using 500 samples unequally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=25m/s 96

Fig. 3.3-5 Effectiveness versus mass flow rate using 150 samples unequally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=12.5m/s 97

Fig. 3.3-6 Effectiveness versus mass flow rate using 150 samples unequally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=25m/s 98

Fig. 3.3-7 Predicted effectiveness using the simple modelversus effectiveness from detailed model for 999 randomly picked points 99

Fig. 3.3-8 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 81 equally spaced training samples, using the approach using no additional knowledge 100

Fig. 3.3-9 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 81 equally spaced training samples, using the approach to correct simple model 101

Fig. 3.3-10 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 500 unequally spaced training samples, using the approach using no additional knowledge 102

Fig. 3.3-11 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 500 unequally spaced training samples, using the approach to correct simple model 103

Fig. 3.3-12 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 150 unequally spaced training samples, using the approach using no additional knowledge 104

Fig. 3.3-13 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 150 unequally spaced training samples, using the approach to correct simple model 104

Fig. 3.3-14 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 81 equally spaced training samples, using the approach using no additional knowledge, allowing 6 wiggles in the wiggle method 106

Fig. 3.3-15 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 81 equally spaced training samples, using the approach using no additional knowledge, allowing 6 wiggles in the wiggle method 107

Fig. 3.3-16 Effectiveness versus mass flow rate using 81 samples equally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=12.5m/s, allowing 6 inflection points in the wiggle method. 109

Fig. 3.3-17 Effectiveness versus mass flow rate using 81 samples equally spaced, plotted for $T_{in,water}$=360K, T_{air}=300K, velocity=25m/s, allowing 6 inflection points in the wiggle method 110

Fig. 3.3-18 Predicted effectiveness versus effectiveness from detailed model for 999 randomly picked points for 150 unequally spaced training samples, allowing more inflections, using the approach using no additional knowledge 111

Fig. 3.3-19 Effectiveness versus mass flow rate using 150 samples unequally spaced, allowing more wiggles, plotted for $T_{in,water}$ =360K, T_{air}=300K, velocity=12.5m/s 112

Fig. 3.3-20 Effectiveness versus mass flow rate using 150 samples unequally spaced, allowing more wiggles plotted for $T_{in,water}$ =360K, T_{air}=300K, velocity=25m/s 113

Fig. 3.4-1 Comparison of prediction using simple model or not, 81 equally spaced training samples, T_{air}=300K, velocity=25m/s 115

Fig. 3.4-2 Procedure to predict under the assumption of independence 117

Fig. 3.4-3 Using no simple model and a temperature correction or not at T_{air}=300K, velocity=25m/s compared to the real effectivenss 118

Fig. 3.4-4 Using simple model and a temperature correction or not at T_{air}=300K, velocity=25m/s compared to the real effectivenss 119

Fig. 3.4-5 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for approach correcting the Temperature dependence for 9 and 9 equally spaced training samples, using the approach to correct simple model 120

Fig. 3.4-6 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for the approach correcting Temperature Dependence with 9 and 9 equally spaced training samples, using the approach without additional knowledge 121

Fig. 3.5-1 Error distribution 124

Fig. 3.5-2 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for 150 unequally spaced training samples including noise, ignoring knowledge about simple model 125

Fig. 3.5-3 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for 150 unequally spaced training samples including noise, using the approach to correct simple model 126

Fig. 3.5-4 Comparison of prediction using simple model or not. 150 unequally spaced training samples including noise, $T_{in,water}$ =360K, T_{air}=300K, velocity=12.5m/s 127

Fig. 3.5-5 Comparison of prediction using simple model or not. 150 unequally spaced training samples including noise, $T_{in,water}$ =360K, T_{air}=300K, velocity=25m/s 128

Fig. 3.5-6 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for 500 unequally spaced training samples including noise, ignoring knowledge about simple model 129

Fig. 3.5-7 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for 500 unequally spaced training samples including noise, using the approach to correct simple model 129

Fig. 3.5-8 Comparison of prediction using simple model or not. 500 unequally spaced training samples including noise, $T_{in,water}$ =360K, T_{air}=300K, velocity=12.5m/s 130

Fig. 3.5-9 Comparison of prediction using simple model or not. 500 unequally spaced training samples including noise, $T_{in,water}$ =360K, T_{air}=300K, velocity=25m/s 131

Fig. 3.5-10 Comparison of prediction using simple model or not. 150 unequally spaced training samples including noise, allowing more inflections, $T_{in,water}$ =360K, T_{air}=300K, velocity=12.5m/s 132

Fig. 3.5-11 Comparison of prediction using simple model or not. 150 unequally spaced training samples including noise, allowing more inflections, $T_{in,water}$ =360K, T_{air}=300K, velocity=25m/s 133

Fig. 3.5-12 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for 150 unequally spaced training samples including noise, allowing more inflections, ignoring knowledge about simple model 134

Fig. 3.5-13 Predicted effectiveness versus effectiveness, calculated with the detailed model for 999 randomly picked points for 150 unequally spaced training samples including noise, allowing more inflections, using simple model 134

Table of tables

Table 3.2-1 Parameters over the range the Heat Exchanger is operated 88

Table 3.3-1 Values for 81 training samples 90

Table 3.6-1 Sum of squares depending on the conditions used for the prediction 136

Foreword

Working on this project that included innovative methods, was a great pleasure for me. I learned more about a field that always interested me. I therefore want to thank everybody who made this possible.

But first a few words about who I am. I came to the University of Wisconsin - Madison in August 1994 being part of an exchange program sponsored by the DAAD, the German Academic Exchange Service. Before I studied Chemical Engineering at the University of Stuttgart in Germany. Very early on in my studies I got introduced to the exchange program with Madison. After may meetings with Professor Zeitz, the managing Professor of the exchange program the first day in Madison finally arrived.

The time in Madison was a very special time for me. I met many different and interesting people. I could study different subjects that interested me for a very long time already. The project I could work on was definitely the climax of my academic life. A project that included investigations in a new field, a project that allowed to do big steps towards a goal but as well a project that taught me that not every step I made was rewarded with success. I am very thankful for each one of the experiences I could make here in the course of this project and in the entire time here in Madison.

A very special thank belongs to Professor Klein, Professor Beckman and Professor Mitchell, who had the idea and the vision to investigate in this field. They made it possible for

me to stay in Madison after the exchange program was over. Professor Klein, Professor Beckman and Professor Mitchell were very helpful by questioning the different approaches made and by challenging me in my work. Their vision brought the work forward.

Professor Zeitz with his experience of running this exchange program for many years was of incredible help before I even left Stuttgart. His insight into what to expect in Madison helped prepare for the time in Madison. Without his help the time before the departure with all the paperwork and beurocratic necessities would have been very difficult. I wish for Professor Zeitz that the future of this exchange program is secure. It is an experience that I do not want to miss and that I hope many more students will be able to have. The work and energy Professor Zeitz puts into this exchange program is remarkable.

The path that many other students sponsored by the DAAD walked on was very easy to follow. The preparation of the DAAD was impressive. It was no problem to get a visa. The DAAD took care of insurance problems and all these little things that are so easy to forget but that are so important for a successful time were taken care of. The work the DAAD does is incredible. Very special thanks belong to the DAAD for the commitment to bring students abroad to experience a different way of studying and a different way of life. The DAAD's commitment to interest students not only in their own field but as well in what is happening around them and to interest them in other cultures. In the light of civil wars over cultural differences, it is more than important that the understanding that despite the cultural differences we are all one people. And that the differences enrich the life and not oppress one's personal

culture. The DAAD provides ground to build on for more acceptance in this world. I hope that it is possible for many more students to go this way.

The friends I found here, in the Graduate Fellowship of Intervarsity Christian Fellowship, the University Community Church and all my other friends I met in the time here in Madison were there when I needed them and I could be there when they needed me. A very special thank belongs to my roommate Andy, whom I lived with for more than a year. Those discussions at two o'clock in the morning about the differences between the US and Germany challenged my insight in each one of the cultures. It helped me not only to understand more about the US but even more to help me understand Germany. Suzy who became a very special friend to me in the past year kept me going at those times when things did not look that good. Suzy tried to explain to me the all so American things. She tried to explain to me why the top ten list of David Letterman is funny, well now I know why, but I still cannot laugh about it. I guess these are things that take longer than sixteen moths to learn.

May be the thank to my parents should have been at the first place. My parents are those two people who probably know me the longest and probably the best too. When I got home from school as a little boy and even now with a new idea how I could change the world, they listened. But they taught me that all change has to start out in my own life first and that little things can create a big change too. My parents raised me in such a way that I could accept the differences of different people. They taught me patience as well as that it is sometimes necessary to work hard in order to achieve a goal. My parents taught me that only

a few things are free in this world, for all the other things you have to work. My parents taught me that seven million two hundred years are not enough to understand ‘live the universe and everything’, they taught me much rather that every little step we make to understand more about the field we work in and every step to understand who we are is worth it. Every little thing in our lives is worth to be thankful for.

The next step after returning to Germany is right ahead, and I am ready to work on it. The preparation I received here, from advisers, friends and from live will help to peruse happiness in what ever is to come.

Thank you everybody for your help!

Matthias M. Bauer