

**Slovak University of Technology in Bratislava
Institute of Information Engineering, Automation, and Mathematics**

PROCEEDINGS

17th International Conference on Process Control 2009

Hotel Baník, Štrbské Pleso, Slovakia, June 9 – 12, 2009

ISBN 978-80-227-3081-5

<http://www.kirp.chtf.stuba.sk/pc09>

Editors: M. Fikar and M. Kvasnica

Vasičkaninová, A., Bakošová, M.: Neural Network Predictive Control of a Chemical Reactor, Editors: Fikar, M., Kvasnica, M., In *Proceedings of the 17th International Conference on Process Control '09*, Štrbské Pleso, Slovakia, 426–431, 2009.

Full paper online: <http://www.kirp.chtf.stuba.sk/pc09/data/abstracts/097.html>

NEURAL NETWORK PREDICTIVE CONTROL OF A CHEMICAL REACTOR

A. Vasičkaninová and M. Bakošová

*Department of Information Engineering and Process Control, Institute of Information Engineering, Automation and Mathematics, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9, 81237 Bratislava, Slovakia
e-mail: {anna.vasickaninova, monika.bakosova}@stuba.sk*

Abstract: Model Predictive Control (MPC) refers to a class of algorithms that compute a sequence of manipulated variable adjustments in order to optimize the future behaviour of a plant. MPC technology can now be found in a wide variety of application areas. The neural network predictive controller that is discussed in this paper uses a neural network model of a nonlinear plant to predict future plant performance. The controller calculates the control input that will optimize plant performance over a specified future time horizon. In the paper the neural network based predictive control for the continuous stirred tank reactor is presented.

Keywords: model predictive control, neural network, continuous stirred tank reactor.

1 INTRODUCTION

Conventional process control systems utilize linear dynamic models. For highly nonlinear systems, control techniques directly based on nonlinear models can be expected to provide significantly improved performance.

Model Predictive Control (MPC) concept has been extensively studied and widely accepted in industry applications. The main reasons for such popularity of the predictive control strategies are the intuitiveness and the explicit constraint handling.

The predictive controllers are used in many areas, where high-quality control is required (Qin and Badgwell, 1996; Qin and Badgwell, 2000; Rawlings, 2000). Model-based predictive control refers to a class of control algorithms, which are based on a process model. MBPC can be applied to such systems as e.g. multivariable, non-minimum-phase, open-loop unstable, non-linear, or systems with a long time delay. Constrained model predictive control becomes the standard algorithm for advanced control in process industries.

Several versions of MPC techniques are Model Algorithmic Control (MAC) (Richalet *et al.*, 1978), Dynamic Matrix Control (DMC) (Cutler and Ramaker, 1980), and Internal Model Control (IMC) (Garcia and Morari, 1982). Although the above techniques differ from each other in some details,

they are fundamentally the same, all of them are based on linear process modelling. If the nonlinear model is available, the computational requirements are expected to be very high (Garcia *et al.*, 1989), especially for nonlinear MIMO processes. It is estimated that, in a typical commissioning project, modelling efforts can take up to 90% of the cost and time in implementing a model predictive controller (Morari and Lee, 1999). There were a number of contributions in the field issues like stability, efficient computation, optimization, constraints and others (Allgöwer and Zheng, 2000; Kouvaritakis and Cannon, 2001; Qin and Badgwell, 2003).

The Neural Network Model Predictive Control (NNMPC) is another typical and straightforward application of neural networks to nonlinear control. When a neural network is combined with MPC approach, it is used as a forward process model for the prediction of process output (Hunt *et al.*, 1992; Nørgaard *et al.*, 2000).

Control of chemical reactors is one of the most studied areas of process control. In this paper, a neural network based predictive control strategy is applied to a continuous-time stirred reactor with two first-order irreversible parallel exothermic reactions. Simulation results show that neural network based predictive control gives promising results.

The paper is organized as follows. Section 2 describes the concept of the model-based predictive

control. Section 3 presents the neural network predictive control strategy and the Levenberg-Marquardt algorithm for selecting the network parameters. In section 4 the continuous stirred tank reactor and Neural Network Model Predictive Control of the reactor is described, simulation results and comparison with PID control are presented and discussed. Finally, in section 5 some concluding remarks are presented.

2 MODEL-BASED PREDICTIVE CONTROL (MBPC)

MBPC is a name for several different control techniques. They all are associated with the same idea. The prediction is based on the model of the process.

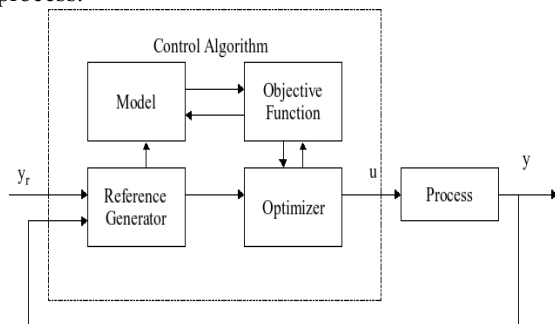


Fig. 1. Classical model-based predictive control scheme

The target of the model-based predictive control is to predict the future behaviour of the process over a certain horizon using the dynamic model and obtaining the control actions to minimize a certain criterion, generally

$$J(k, u|k) = \sum_{j=N_1}^{N_2} (y(k+j) - y_r(k+j))^2 + \lambda \sum_{j=1}^{N_u} (u(k+j-1))^2 \quad (1)$$

Signals $y(k+j)$, $y_r(k+j)$, $u(k+j)$ are j -step ahead predictions of the process output, the reference trajectory and the control signal, respectively. The values N_1 and N_2 are minimal and maximal prediction horizons and N_u is the prediction horizon of control signal. The value of N_2 should cover the important part of the step response curve. The use of the control horizon N_u reduces the computational load of the method. The parameter λ represents the weight of the control signal. At each sampling period only the first control signal of the calculated sequence is applied to the controlled process. At the next sampling time the procedure is repeated. This is known as the receding horizon concept.

The controller consists of the plant model and the optimization block.

Eq. (1) is used in combination with input and output constraints:

$$\begin{aligned} u_{min} &\leq u \leq u_{max} \\ \Delta u_{min} &\leq \Delta u \leq \Delta u_{max} \\ y_{min} &\leq y \leq y_{max} \\ \Delta y_{min} &\leq \Delta y \leq \Delta y_{max} \end{aligned} \quad (2)$$

The ability to handle constraints is one of the key properties of MBPC and also caused its spread, use, and popularity in industry.

MBPC algorithms are reported to be very versatile and robust in process control applications.

3 NEURAL NETWORK PREDICTIVE CONTROL

Neural networks have been applied very successfully in the identification and control of dynamic systems. The universal approximation capabilities of the multilayer perceptron make it a popular choice for modelling of nonlinear systems and for implementing of nonlinear controllers.

The unknown function may correspond to a system we are trying to control, in which case the neural network will be the identified plant model.

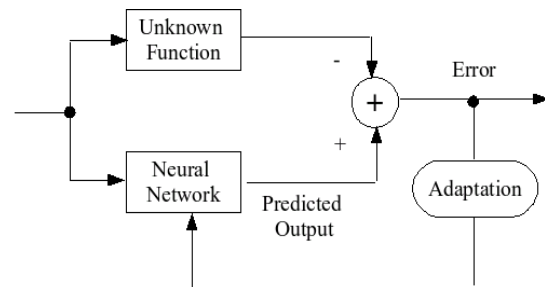


Fig. 2. Neural network as a function approximator

Two-layer networks, with sigmoid transfer functions in the hidden layer and linear transfer functions in the output layer, are universal approximators (Figure 2).

The prediction error between the plant output and the neural network output is used as the neural network training signal. The neural network plant model uses previous inputs and previous plant outputs to predict future values of the plant output. The structure of the neural network plant model is given in the following figure, where $u(k)$ is the system input, $y_p(k)$ is the plant output, $y_m(k)$ is the neural network model plant output, the blocks labelled TDL are tapped delay lines that store previous values of the input signal, $I\mathbf{W}^{i,j}$ is the weight matrix from input number j to layer number i . $L\mathbf{W}^{i,j}$ is the weight matrix from layer number j to layer number i .

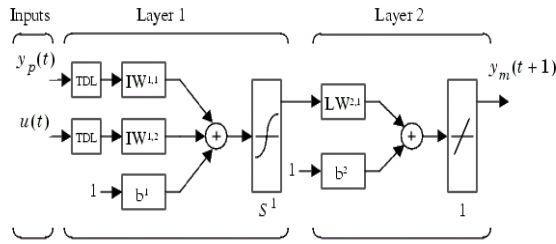


Fig. 3. Structure of the neural network plant model

This network can be trained off-line in batch mode, using data collected from the operation of the plant.

The procedure for selecting the network parameters is called training the network. The Levenberg-Marquardt (LM) algorithm is very efficient for training. The LM algorithm is an iterative technique that locates the minimum of a function that is expressed as the sum of squares of nonlinear functions. It has become a standard technique for nonlinear least-squares problems and can be thought of as a combination of steepest descent and the Gauss-Newton method (Levenberg, 1944; Madsen *et al.*, 2004; Marquardt, 1963; Mittelmann, 2004, Kelley, 1999).

When the current solution is far from the correct one, the algorithm behaves like a steepest descent method: slow, but guaranteed to converge. When the current solution is close to the correct solution, it becomes a Gauss-Newton method.

Let f be an assumed functional relation which maps a parameter vector $p \in R^m$ to an estimated measurement vector $\hat{x} = f(p)$, $\hat{x} \in R^n$. An initial parameter estimate p_0 and a measured vector x are provided and it is desired to find the vector p^+ that best satisfies the functional relation f , i.e. minimizes the squared distance $e^T e$ with $e = x - \hat{x}$. The basis of the LM algorithm is a linear approximation to f in the neighbourhood of p . For a small $\|\delta_p\|$, a Taylor series expansion leads to the approximation $f(p + \delta_p) \approx f(p) + J\delta_p$ where J is the Jacobian matrix $\frac{\partial f(p)}{\partial p}$. Like all non-linear optimization methods, LM is iterative: initiated at the starting point p_0 , the method produces a series of vectors p_1, p_2, \dots , that converge towards a local minimizer p^+ for f . Hence, at each step, it is required to find the δ_p that minimizes the quantity $\|e - J\delta_p\|$. The sought δ_p is thus the solution of a linear least-square problem: the minimum is attained when $J\delta_p - e$ is orthogonal to the column space of J . This leads to $J^T(J\delta_p - e) = 0$, which yields δ_p as the solution of the normal equations:

$$J^T J \delta_p = J^T e. \quad (3)$$

The matrix $J^T J$ in the left hand side of Eq. (3) is the approximate Hessian, i.e. an approximation to the matrix of second order derivatives. The LM method actually solves a slight variation of Eq. (3), known as the augmented normal equations $N\delta_p = J^T e$,

where the off-diagonal elements of N are identical to the corresponding elements of $J^T J$ and the diagonal elements are given by $N_{ii} = \mu + [J^T J]_{ii}$ for some $\mu > 0$. The strategy of altering the diagonal elements of $J^T J$ is damping and μ is referred to the damping term. If the updated parameter vector $p + \delta_p$ with δ_p computed from Eq. (3) leads to a reduction of the error e , the update is accepted and the process repeats with a decreased damping term. Otherwise, the damping term is increased, the augmented normal equations are solved again and the process iterates until a value of δ_p that decreases error is found.

In LM, the damping term is adjusted at each iteration to assure a reduction in the error e . The LM algorithm terminates when at least one of the following conditions is met:

1. The magnitude of the gradient of $e^T e$, i.e. $J^T e$ in the right hand side of Eq. (3), drops below a threshold ϵ_1 .
2. The relative change in the magnitude of δ_p drops below a threshold ϵ_2 .
3. The error $e^T e$ drops below a threshold ϵ_3 .
4. A maximum number of iterations k_{max} is completed.

If a covariance matrix Σ for the measured vector x is available, the minimum is found by solving a weighted least squares problem defined by the weighted normal equations

$$J^T \Sigma J \delta_p = J^T \Sigma e \quad (4)$$

4 SIMULATIONS AND RESULTS

4.1 Chemical reactor

Consider a chemical reactor (Vasičkaninová and Bakošová, 2005; Vasičkaninová and Bakošová, 2006) with first-order irreversible parallel reactions according to the scheme $A \xrightarrow{k_1} B$ $A \xrightarrow{k_2} C$. The measured output is temperature of the reaction mixture.

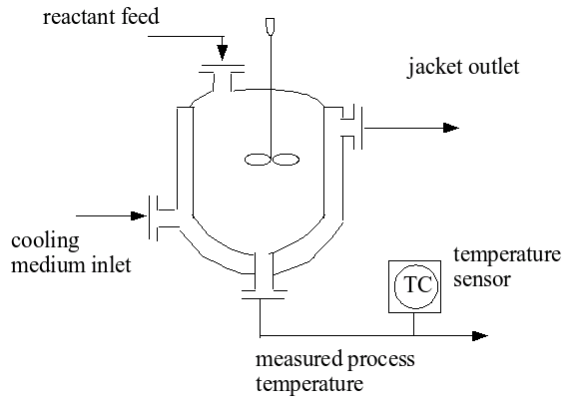


Fig. 4. Jacketed continuous stirred tank reactor
The simplified non-linear dynamic mathematical model of the chemical reactor consists of five differential equations:

$$\frac{dc_A}{dt} = \frac{q}{V} c_{Av} - \frac{q}{V} c_A - k_1 c_A - k_2 c_A \quad (5)$$

$$\frac{dc_B}{dt} = \frac{q}{V} c_{Bv} - \frac{q}{V} c_B + k_1 c_A \quad (6)$$

$$\frac{dc_C}{dt} = \frac{q}{V} c_{Cv} - \frac{q}{V} c_C + k_2 c_A \quad (7)$$

$$\frac{dT}{dt} = \frac{q}{V} T_v - \frac{q}{V} T - \frac{Ak}{V\rho C_p} [T - T_c] + \frac{\dot{Q}_r}{V\rho C_p} \quad (8)$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c} T_{vc} - \frac{q_c}{V_c} T_c + \frac{Ak}{V_c \rho_c C_{pc}} [T - T_c] \quad (9)$$

The reaction rate coefficients are non-linear functions of the reaction temperature being defined by the Arrhenius relations

$$k_1 = k_{10} e^{-\frac{E_1}{RT}} \quad k_2 = k_{20} e^{-\frac{E_2}{RT}} \quad (10)$$

The heat generated by chemical reactions is expressed as

$$\dot{Q}_r = k_1 c_A V (-\Delta_r H_1) + k_2 c_A V (-\Delta_r H_2) \quad (11)$$

Here, c are concentrations, T are temperatures, V are volumes, r are densities, C_p are specific heat capacities, q are volumetric flow rates, $\Delta_r H$ are reaction enthalpies, A is the heat transfer area, k is the heat transfer coefficient. The subscript c denotes the coolant, r the reacting mixture and the superscript s denotes the steady-state values in the main operating point. Parameters and inputs of the reactor are enumerated in Table 1.

Table 1. Reactor parameters and inputs

Variable	Unit	Value
q	$\text{m}^3 \text{min}^{-1}$	0.015
V	m^3	0.23
V_c	m^3	0.21
ρ	kg m^{-3}	1020

Variable	Unit	Value
ρ_c	kg m^{-3}	998
C_p	$\text{kJ kg}^{-1} \text{K}^{-1}$	4.02
C_{pc}	$\text{kJ kg}^{-1} \text{K}^{-1}$	4.182
A	m^2	1.51
k	$\text{kJ m}^{-2} \text{min}^{-1} \text{K}^{-1}$	42.8
k_{10}	min^{-1}	$1.55 \cdot 10^{11}$
k_{20}	min^{-1}	$4.55 \cdot 10^{25}$
E_1/R	K	9850
E_2/R	K	22019
$\Delta_r H_1$	kJ kmol^{-1}	$-8.6 \cdot 10^4$
$\Delta_r H_2$	kJ kmol^{-1}	$-1.82 \cdot 10^4$
c_{Av}	kmol m^{-3}	4.22
c_{Bv}	kmol m^{-3}	0
c_{Cv}	kmol m^{-3}	0
U_v	K	328
U_{cv}	K	298
q_c^s	$\text{m}^3 \text{min}^{-1}$	0.004
T^s	K	363.61
T_c^s	K	350.15
c_A^s	kmol m^{-3}	0.4915
c_B^s	kmol m^{-3}	2.0042
c_C^s	kmol m^{-3}	1.7243

The reactions in the described reactor are exothermic ones and the heat generated by the chemical reactions is removed by the coolant in the jacket of the tank. The control objective is to keep the temperature of the reacting mixture close to a desired value.

4.2 Neural Network Model Predictive Control

The controller uses a neural network model to predict future plant responses to potential control signals. An optimization algorithm then computes the control signals that optimize future plant performance. The neural network plant model is trained off-line, in batch form, using any of the training algorithms. The controller, however, requires a significant amount of online computation, because an optimization algorithm is performed at each sample time to compute the optimal control input.

The model predictive control method is based on the receding horizon technique. The neural network model predicts the plant response over a specified time horizon. The predictions are used by a numerical optimization program to determine the control signal that minimizes the following performance criterion over the specified horizon.

$$J(k, u(k)) = \sum_{j=N_1}^{N_2} (y_m(k+j) - y_r(k+j))^2 + \lambda \sum_{j=1}^{N_u} (u'(k+j-1) - u'(k+j-2)) \quad (12)$$

where N_1 , N_2 , and N_u define the horizons over which the tracking error and the control increments are evaluated. The u' variable is the tentative control signal, y_r is the reference response, and y_m is the network model response. The λ value determines the

contribution that the sum of the squares of the control increments has on the performance index (Demuth and Beale, 2002). The controller block is implemented in Simulink. Constraints and parameters values: $0 \leq u \leq 0.02$, $354 \leq y_p \leq 365$, $N_1=1$, $N_2=7$, $N_u=3$, $\lambda=0.5$.

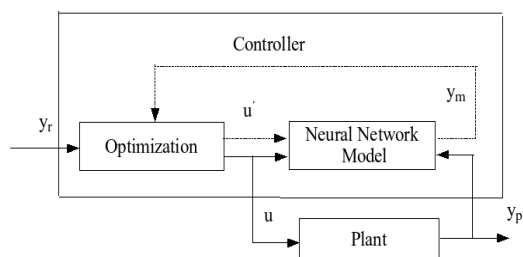


Fig. 5. Neural Network Predictive Control

The feedback PID controllers were tuned by various methods (Ogunnaiké and Ray, 1994) and the best simulation results were obtained with PID controller tuned using Chien-Hrones-Reswick method and its parameters are $K_C = -0.003$, $T_I = 16.8$, $T_D = 1.41$.

In Figure 6 the predictive control of the reacting mixture temperature in comparison with PID control and the reference trajectory are shown.

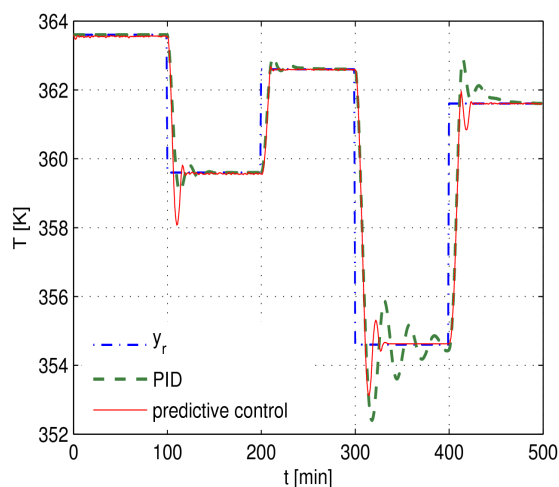


Fig. 6. Comparison of neural network predictive control of a CSTR with PID control.

The step changes of the reference y_r were generated and the MBP and PID controllers were compared using the well-known iae and ise criteria described as follows:

$$iae = \int_0^T |e| dt \quad (13)$$

$$ise = \int_0^T e^2 dt \quad (14)$$

The iae and ise values are given in Table 4.

Table 4: Comparison of the simulation results by integrated absolute error and integrated square error.

control method	iae	ise
predictive control	174	707
PID controller	219	770

5 CONCLUSIONS

In this paper, a neural network based predictive control strategy is applied to a continuous-time stirred reactor with two first-order irreversible parallel exothermic reactions. Chemical reactors with exothermic reactions represent the most dangerous operational units in the chemical industry. The simulation results confirmed that neural network based predictive control is one of the possibilities for successful control of CSTRs. The advantage of this approach is that it is not linear-model-based strategy and the control input constraints are directly included to the synthesis. Comparison of the MBPC simulation results with classical PID control demonstrates the effectiveness and superiority of the proposed approach.

ACKNOWLEDGMENTS

The work has been supported by the Scientific Grant Agency of the Slovak Republic under grants 1/4055/07, 1/0071/09 and by the Slovak Research and Development Agency under the project APVV-0029-07.

6 REFERENCES

- Allgöwer, F. and Zheng A. (Eds.). (2000). *Nonlinear Model Predictive Control*, Progress in system and control theory, **26**, Birkhäuser Verlag, Basel.
- Cutler C. R. and Ramaker. (1980). Dynamic matrix control - a computer control algorithm. *Proc. Amer. Control Conf.*, WP5-B
- Demuth, H. and M. Beale. (2002). Neural Network Toolbox For Use with MATLAB®. Control Systems. 205-242. URL http://www.image.ece.ntua.gr/courses_static/nn/matlab/nnet.pdf.
- Garcia C. E. and M. Morari. (1982). Internal model control-I. A unifying review and some new results. *Ind. Eng. Chem. Process Des. Dev.* **21**, 308--323.
- Garcia C. E., D. M. Prett and M. Morari. (1989). Model predictive control, theory and practice-a survey. *Automatica* **25**(3), 335-348.

- Hunt K. J., D. Sbarbaro, R. Zbikowski and P. J. Gawthrop. (1992). Neural networks for control systems-A survey. *Automatica* **28**(6), 1083-1112.
- Kelley, C. T. (1999). Iterative Methods for Optimization. SIAM Press, Philadelphia.
- Kouvaritakis B., Cannon M. (Eds.). (2001). Nonlinear predictive control, Theory and practice, *IEE Control Engineering Series* 61, IEE.
- Levenberg, K. (1944). A Method for the Solution of Certain Non-linear Problems in Least Squares, *Quarterly of Applied Mathematics*, **2**(2), 164-168.
- Madsen, K., H.B. Nielsen and O. Tingleff (2004). Methods for Non-Linear Least Squares Problems. Technical University of Denmark, Lecture notes, Available: <http://www.imm.dtu.dk/courses/02611/nllsq.pdf>.
- Marquardt, W. (1963). An Algorithm for the Least-Squares Estimation of Nonlinear Parameters. *SIAM Journal of Applied Mathematics*, **11**(2), 431-441.
- Mittelmann, D. (2004). The Least Squares Problem. Available: <http://plato.asu.edu/topics/problems/nllsq.html>.
- Morari, M. and J. H. Lee. (1999). Model predictive control: past, present and future, *Computers and Chemical Engineering*, **23**, 667-682.
- Nørgaard, M., O. Ravn, N. K. Poulsen and L. K. Hansen. (2000). *Neural networks for modelling and control of dynamic systems*, Springer, London
- Ogunnaike, B. A. and Ray, W. H. (1994). *Process Dynamics, Modelling, and Control*. 536-541. Oxford University Press. New York. 1259. ISBN 0-19-509119-1.
- Qin S. J. and Badgwell T. A. (1996). An overview of industrial model predictive control technology. *Fifth International Conference on Chemical Process Control - CPC V*, 232-56. American Institute of Chemical Engineers.
- Qin S. J. and Badgwell T. A. (2000). An overview of nonlinear model predictive control applications. *Nonlinear Predictive Control*, 369-393. Birkhäuser.
- Qin S. J. and Badgwell T. A. (2003). A survey of industrial model predictive control technology. *Contr. Eng. Pract.*, **7**(11), 733 -764.
- Rawlings J. B. (2000). Tutorial overview of model predictive control. *IEEE Contr. Syst. Magazine*, **20**(3), 38-52.
- Richalet J. A., A. Rault, J. D. Testud and J. Papon. (1978). Model predictive heuristic control: applications to an industrial process. *Automatica* **14**, 413-428.
- Vasičkaninová, A. and M. Bakošová. (2005). Cascade fuzzy logic control of a chemical reactor. In *Proc. 15. Int. Conference Process Control '05*, Štrbské Pleso, High Tatras.
- Vasičkaninová, A. and M. Bakošová. (2006). Fuzzy modelling and identification of the chemical technological processes. In *Proc. 7. Int. Scientific-Technical Conf. Process Control 2006*, University of Pardubice, Kouty nad Desnou.
- Neural Network Toolbox™ - Getting Started Guide, The MathWorks, 2008