15 Modeling and Optimizing a Recipe for a Paint Coating

learning objectives:

- factors involved in adjusting an industrial recipe (ingredients plus processing conditions) while maintaining consistent results
- identification of controlling variables as **little correlated** with each other as possible
- use of experiments to select training data
- comparison of 3-D and 2-D (sectioned) display of the results: **partial models**

15.1 The Problem

This example is a typical industrial application of modeling. The chemical, pharmaceutical, food, and many other industries rely heavily on recipes for their products. A recipe usually consists of two types of quantities: the first comprises the amounts of components that should be put together or processed; the second type consists of process parameters, like temperature of processing, *pH* of solvent, time of mixing, etc., necessary to make the ingredients into a product.

In order to maintain preset levels of quality and/or price, the recipe must be followed exactly; but components may change in price, or suppliers may change **their** products, and all such difficulties require an adjustment of the recipe.

If, for example, the *pH* of the process is critical, then the recipe will have to be adjusted if some component from a new supplier has a higher or lower acidity; and adjusting the quantity of one component probably calls for adjustments of all other components to maintain consistent properties and quality of the product.

Recipes are as delicate as complex circuits; adjusting one is often considered an "art", since an analytical dependence of product properties on compound properties (and on component **interactions**) is unknown.

> Remember that there are **multiple** product properties that must be kept within prescribed tolerances.

We want to find a non-analytical means of adjusting the conditions and ingredient quantities to bring product properties back within specs; and if this is not possible, the method should tell us **that**, too.

15.2 The Data

The example that will be followed here was worked out by Tusar and coworkers at the National Institute of Chemistry in Ljubljana, Slovenia, for a chemical factory which produces different kinds of paints, paint coatings, and related products. The goal was to obtain full knowledge about the dependencies among the various properties (coordinates in measurement space) of a product that we will call simply "paint coating".

During intensive studies of this product, it was found that there are three highly significant and **non-correlated** (or only slightly correlated) variables: concentration of the polymer component, C_p, concentration of the catalyst, C_c, and the temperature T used for heating the product. Six properties have to be controlled and adjusted to the norms for this product:

- hardness, H
- elasticity, E
- adhesiveness, A
- resistance to *methyl-isobutyl-ketone*, *MIBK*
- stroke resistance, *SR*
- contra-stroke resistance, *CSR*

Using standard modeling techniques, six models are set up:

$$H = f_1 (C_p, C_c, T, a_h, b_h, c_h, ...)$$

$$E = f_2 (C_p, C_c, T, a_e, b_e, c_e, ...)$$

$$A = f_3 (C_p, C_c, T, a_a, b_a, c_a, ...)$$

$$
\begin{aligned}
MIBK &= f_4\,(C_p, C_c, T, a_{mibk}, b_{mibk}, c_{mibk}, \ldots)\\
SR &= f_5\,(C_p, C_c, T, a_{sr}, b_{sr}, c_{sr}, \ldots) \qquad (15.1)\\
CSR &= f_6\,(C_p, C_c, T, a_{csr}, b_{csr}, c_{csr}, \ldots)
\end{aligned}
$$

This means that we need to invent (or guess!) functions $f_1, f_2, \ldots, f_6$ that give values of these six properties in terms of the three controlling variables. Furthermore all six sets of adjustable coefficients $a_k, b_k, c_k, \ldots$ should be determined in such a way that the set of experimental values $\{H_s, E_s, A_s, MIBK_s, SR_s, CSR_s\}$ will fit the set of calculated ones at given values of $\{C_{sp}, C_{sc}, T_s\}$ as well as possible.

As we already know, supervised neural network learning does not require any prior assumptions or hypotheses about the function types, numbers of parameters, etc. All that is needed is a well selected architecture and the input data and targets to which the model should be adapted.

The data for the model were selected using a full three-variable three-level experimental design requiring 27 measurement points (Figure 15-1).

Accordingly, 27 cover paints were made in the test laboratory and for each paint all 6 properties were measured. Altogether a matrix of 27 x (3 + 6) = 243 values was obtained: 81 were used as input vectors (27 x 3) and 162 as targets (27 x 6). A few of the experiments used in developing the model are given in Table 15-1; output values in this Table are given on a quality scale, on which 1.0 represents superior quality, while values represented by 0.0 actually mean that the measured property is so bad that it may not even be measurable.

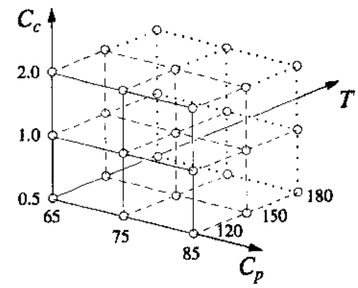

Figure 15-1: Full three-variable, three-level experimental (factorial) design for determining the dataset for training and testing the model.

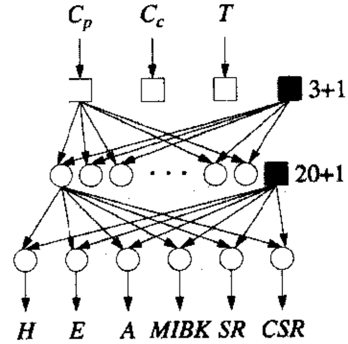

Figure 15-2: (3 + 1) x (20 + 1) x 6 neural network for modeling properties of paint coatings.

15.3 The Network and Training

As usual in our examples, a one-hidden-layer neural network was chosen, having three input units, six output neurons, 20 neurons in the hidden layer, and 189 weights (Figure 15-2).

The 81 input values were normalized between 0 and 1, while the 162 output values were additionally scaled into the interval 0.2 – 0.8. This further scaling is often recommended for output neurons having a nonlinear squashing function (Equation (2.39)), but trained to yield nearly linear outputs (Figure 8-15). After about ten thousand epochs, the network became stabilized.

	input			output					
	C_p [%]	C_c [%]	T [°C]	H	E	A	$MIBK$	SR	CSR
1	65	1.0	150	1.0	0.3	0.0	1.0	0.0	0.0
2	65	2.4	150	0.0	0.7	0.8	1.0	0.7	1.0
3	75	0.2	150	1.0	0.9	1.0	1.0	0.0	0.0
4	75	1.0	120	0.5	1.0	0.9	0.9	0.6	0.6
5	75	1.0	150	1.0	0.9	1.0	1.0	0.7	0.8
6	75	1.0	180	1.0	0.9	1.0	1.0	0.0	0.0
7	75	2.4	150	1.0	0.8	0.3	0.8	1.0	0.5
8	85	0.2	150	0.0	1.0	1.0	0.0	1.0	1.0
9	85	2.4	120	0.0	1.0	1.0	0.0	1.0	1.0

Table 15-1: Some of the experiments used for building the model. The output properties are normalized between zero and one: 1.0 signifies an excellent value of the property, while 0.0 represents a bad (or unmeasurable) value.

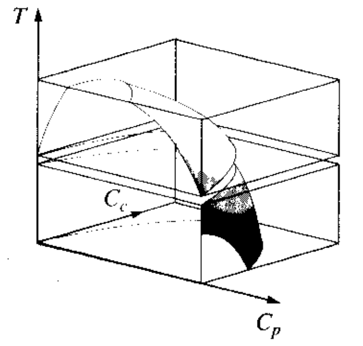

Figure 15-3: Three-dimensional display of surface presenting possible values of the predicted property H. A cut is made at a specific temperature and the two "boxes" have slightly been moved apart for better visualization.

15.4 The Models

We can obtain a separate (partial) model from each of the six outputs. In other words, the signal at each one of the six output neurons can be taken as a substitute for one of the explicit equations given in (15.1). An essential point of this example is that, as always, the models are obtained without any *a priori* knowledge about the behavior of the system.

Because each property (output variable) is a relatively simple function of only three input variables, it can be visualized as a plot in a three-dimensional space comprising variables C_p, C_c and T (Figure 15-3). Unfortunately, when looking at this figure, it becomes clear that only one variable (one surface) can be shown on one such picture.

However, even this three-dimensional display does not offer more than a qualitative description of the property behavior. In order to get usable quantitative output, we must produce two-dimensional maps (each at a constant value of the third parameter). Such cross-sectional planes are shown in Figure 15-4; once the model is obtained, these may be drawn at any value of the third variable.

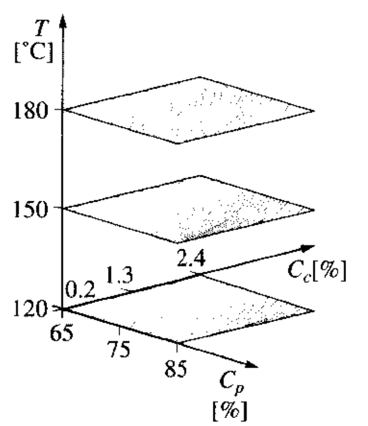

Figure 15-4: Three two-dimensional cross-sections describe the property H better than the three-dimensional surface in Figure 15-3.

The 18 maps in Figure 15-5 show how each of the controlled properties H, E, A, $MIBK$, SR, or CSR behaves. The three maps under each output are only three of many possible constant-T cross-sections.

As discussed above, an analogous map at any temperature between 150°C and 180°C can be obtained at any of the six outputs. These 18 maps illustrate the richness of information that can be obtained from the trained network.

This can easily be programmed on a personal computer, a simple user interface added and the whole package handed over to engineers for use. Since the calculation of all six properties from any triplet of variables C_p, C_c and T can be made almost instantaneously, the entire measurement space can be thoroughly inspected.

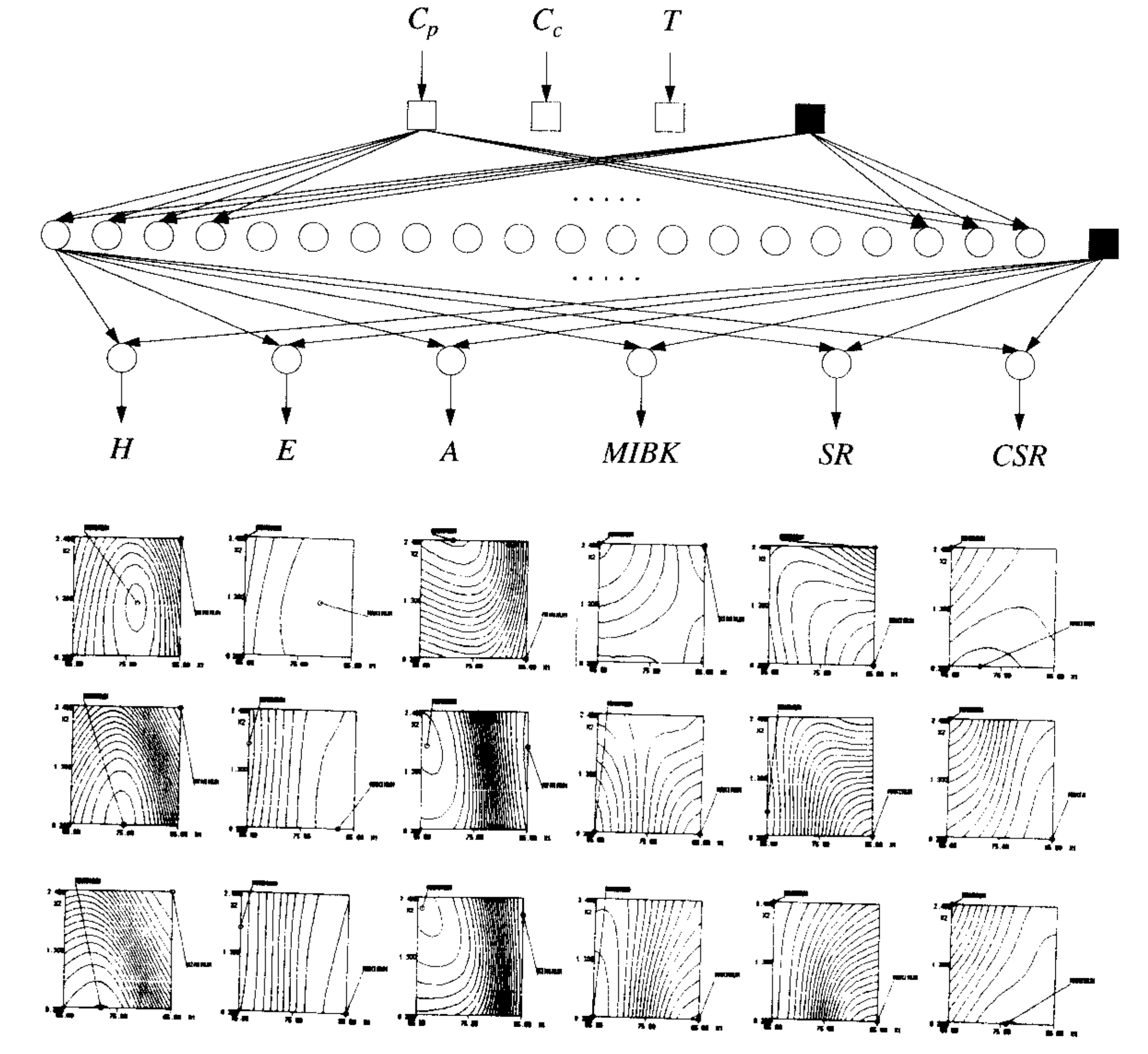

Figure 15-5: Two-dimensional sections through the 3-D input space. Each column of three maps shows the dependance of the indicated output property (H, E, etc.) upon C_p (abscissa) and C_c (ordinate); each map is at a different constant value of T.

15.5 References and Suggested Readings

15-1. L. Tusar, M. Tusar and N. Leskovsek, "A Comparitative Study of Polynominal and Neural Network Modelling for Optimization of Clear Coat Formulations", *Surf. Coat. Intern.* **78** (1995) 427 – 434.

15-2. N. Leskovsek, L. Tusar and M. Tusar, "Empirical Modeling of Rheological and Mechanical Properties of Paint", *Rheology* **5** (1995) 140 - 145.

15-3. M. Tusar, L. Tusar, N. Barle, N. Leskovsek and M. Kumaven, "A Study of the Influence on the Hiding Power of the Composition of a Paint and its Film Thickness", *Surf. Coat. Intern.* **78** (1995) 473 – 479.

15-4. A. P. de Weijer, L. Buydens, G. Kateman and H. M. Heuvel, "Neural Networks Used as a Soft Modeling Technique for Quantitative Description of the Relation Between Physical Structure and Mechanical Properties of Poly(ethylene terephthalate) Yarns", *Chem. Intell. Lab. Systems* **16** (1992) 77 – 86.

15-5. A. P. de Weijer, C. B. Lucasius, L. Buydens, G. Kateman and H. M. Heuvel "Using Genetic Algorithms for an Artificial Neural Network Model Inversion", *Chem. Intell. Lab. Systems* **20** (1993) 45 – 55.