



Review of Machine Learning and **Experimental Design** Īn **Rubber Compounding**

Dr. Hans-Joachim Graf, H-JG Consulting



Content of this Presentation

- Introduction
 - \circ What is Design of Experiments (DoE)
 - What is Artificial Intelligence Software
- Analysis of Data for Predictions with Software "Feed Forward AI"
 - **O DOE (Design of Experiments) Prediction Tool**
 - $\,\circ\,$ Analysis of Data with Al Software
- The Problem with Recurrent AI Software
- Conclusion







- The (statistical) design of experiments (DOE) is an efficient procedure for planning experiments so that the data obtained can be analyzed to yield valid and objective conclusions. ... An Experimental Design is the laying out of a detailed experimental plan in advance of doing the experiment.
- Statistic is a formal science, whose methods are applied to a wide variety of natural and engineering sciences. The interpretation of the results only make sense if they have been verified for their plausibility in the context of the intrinsic sciences.
- In engineering, it is often necessary to work with small samples, so the treatment of small samples or series of experiments and the presentation of distribution-independent test procedures is of particular importance.

Steps of Design of Experiments



Source: T. Duever; UofWaterloo

• An investigation consists of the following steps applied in a <u>sequential</u>, <u>iterative</u> manner:

$\bigcirc \textbf{HYPOTHESIZE}$

○ **DESIGN**

\circ ANALYZE

• The statistic analysis answers the question whether test results are to be considered as random phenomena or may be treated as characteristic.



Regression Analysis

Experimentation: Variation of Factors



Measurements: Responses

$$\rightarrow$$
 R₁, R₂,...R_r

Objective of the Experiment is the identification of the factors $(F_{1,}..F_{n})$ type of influence on the responses $(R_{1,}...R_{n})$ and description with mathematical equations for further processing. ANOVA is used for statistical evaluation.

$$R_{i(1...n)} = f(A_0 + A_1F_1 +A_nF_n +)$$

EPDM Curative study Predicted vs. Actual Predicted vs. Actual Section

TB (Tensile at Break): Predicted over actual, top – linear, bottom – 2FI

DoE: Point Prediction



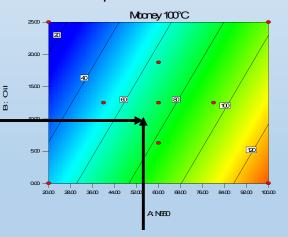
Source: Cabot TB RG-133

Properties of Compound is determined by Polymer, CB and Oil content and the ratio of CB and Oil. Data of DoE converted into a contour plot

- CB 550: 55 phr
- Oil: 10 phr
- Mooney Viscosity: 71 M-Units
- Hardness: 60 ° ShA
- Tensile: 21 MPa
- Elongation: 460 %
- C-Set: 28%

NR Compound

SMR 5CV – 100 phr
 CB – Var
 Oil – Var
 ZnO – 5 phr
 StAc – 1 phr
 AO – 1 phr
 NR 100 phr
 MBTS – 0.6
 S – 2.5 phr

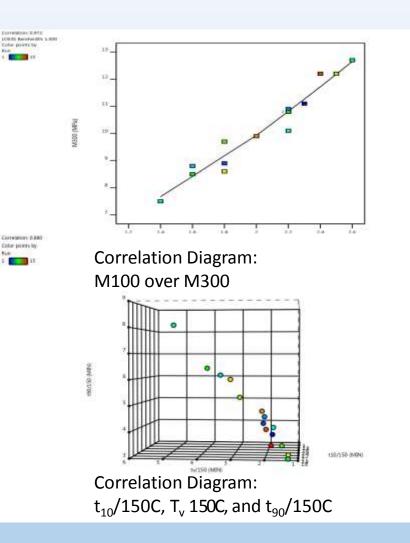




DoE: Tools in Modern DoE Software

Statistic experimental design software tools in Design Expert[®]

- Correlation diagrams allowing a first evaluation of the data:
 - Following inherent logic of rubber principles
- Histograms
- Scatter plots
- Further tools are
 - $\circ \quad \text{Contour plots} \quad$
 - Desirability plots, whether target is met / or failed
 - \circ **Prediction**





DoE: Point Prediction based on Regression

The Prediction is calculated with the

- \circ Intercepts and
- **Regression Factors:**

(Table shows case for linear regression)

Response	Intercept	F1	F2	Fn
R1	A ₁	A _{F1.1}	A _{F2.1}	A _{Fn.1}
R2	A ₂	A _{F1.2}	X _{F2.2}	A _{Fn.2}
Rn	A _n	A _{F.n}	A _{Fn.n}	A _{Fn.n}

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Point Prediction Tool in Design Expert[®]12 Software (Screen shot)



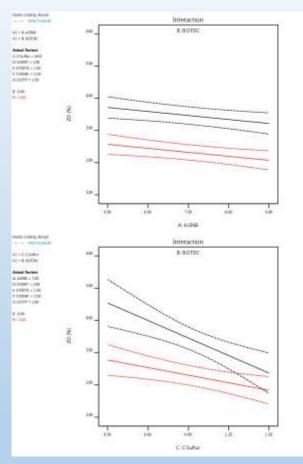
DoE: Advantages and Limits

Advantage

- \odot Investigation of New, Unknown Material
- $\ensuremath{\circ}$ Results are statistically sound
- \odot Estimation of Measurement Error
- $\ensuremath{\circ}$ Identification of Outliers
- \odot Possibility to Schedule and Budget Development

Disadvantage

- Limited Number of Factors in a Compound
 - 3 4 Factors preferred
- \odot Effect of Variation of Factors among themselves
- \odot Extrapolation not recommended
- \odot Results are limited to the compound used for evaluation



TB: Interaction Graph: TB over Sulfur: DTDC top – linear, bottom – 2FI

AI: Random Datasets





Definition: Artificial Intelligence

- The theory and development of computer systems able to perform tasks normally requiring human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages. (google 15.10.21)
- Deep learning, meanwhile, is a subset of machine learning that enables computers to solve more complex problems.
- Neural networks, also known as artificial neural networks (ANNs) or simulated neural networks (SNNs), are a subset of machine learning and are at the heart of deep learning algorithms. Their name and structure are inspired by the human brain, mimicking the way that biological neurons signal to one another.

AI: Random Datasets



Source: G Roden; Heise Medien 2021

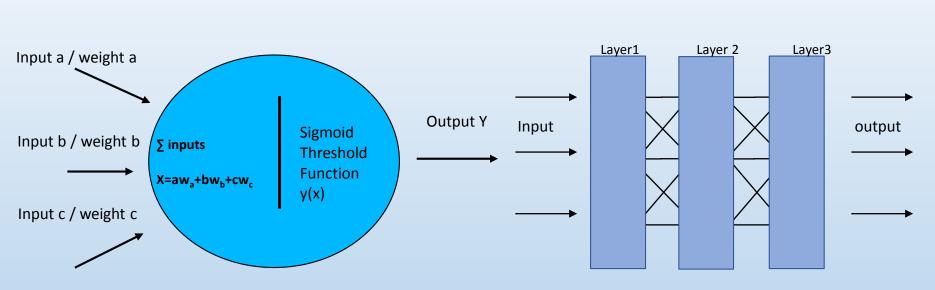
Algorithm used in Al Programming

- k-Means-Algorithm
 - Creates cluster, calculates mean (Centroid) reorganization, Iteration
- > Genetic Algorithm
 - **Proposed Solution**, iteration and mutation towards optimum, selection of results with "fitness" function
- Neuronal Net
 - Complex algorithm (Neuron): Calculation of a weighted sum, normalization to emphasize or dampen the summands. "Input – Hidden – Output" layer.
 Feed Forward Networks / Recurrent Neuronal Networks

AI: Schematic Structure



Source: T. Rashid, Neuronal Nets, 2017



Artificial Intelligence: Neuronal Network and Algorithm

Extended model of an artificial neuron with moderated input weights

A model with multiple layers of neurons, each connected to the preceding and succeeding layer.

 Weights could be assigned to the connections between nodes

AI: Basic Algorithm



Source: T. Rashid, Neuronal Nets, 2017

Matrix multiplication with the terminology of neuronal nets (w - weight, I = Input, O - X-Matrix multiplied sigmoid function)

 $\begin{bmatrix} I & 1 \\ I & 2 \end{bmatrix} \begin{bmatrix} w & 1,2 & w & 2,1 \\ w & 1,2 & w & 2,2 \end{bmatrix} = \begin{bmatrix} I & 1 & *w & 1,1 & I & 2 & *w & 2,1 \\ I & 2 & *w & 1,2 & I & 2 & *w & 2,2 \end{bmatrix}$

The input values for the subsequent layer is in each case:

X = w * I

Each x must be treated with the sigmoid, respective activation function:

 $Y = 1/(1+e^{-x})$

Values for subsequent layers change to: **O** = sigmoid (**X**)

AI: Old Algorithm on Fast Computers



Source: T. Rashid, Neuronal Nets, 2017

Basic Idea of Neuronal Network Calculation:

- The calculation of signals passing through a neural network can be modeled as a matrix calculation.
- The links can be specified more precisely independent of the size of the network.
- Programming languages designed for matrix calculations can perform such calculations efficiently and quickly.
- Calculation speed on todays Machines is fast and able to handle large amounts to calculations in mill seconds

AI: Rubber Compound Formula



Properties

Rubber Recipe Data Stag

- > Ingredients
 - Normalized to 100 parts polymer = phr
- Properties
 - Rheological properties
 - Physicals
 - \circ Other
 - \circ Appearance
 - Dynamics

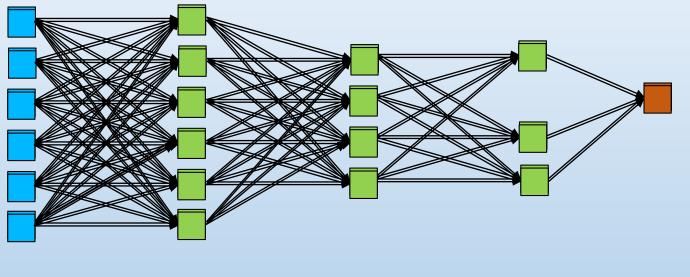
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Fill, Ellit, Degram, Hall

Feed Forward AI Program



A square represents one dataset = data stag consist of n data: upper stage – Ingredients; lower stage - properties



Input 1. Layer n.th Layer n.th + 1 Layer Output

Each square represents recipe and property information

- □ Solutions closer to targets survive
 - □ Walking gradient method

Feed Forward AI Program

Database

(Historic, most likely incomplete, unorganized Data)

Input: Data + Multi target query

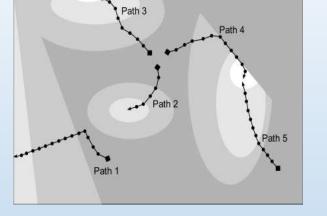
- Search for the best compromise with K-Mean / Multi Objective Evolutionary Algorithm (MOEA)
- Numerical Solution with a "Gradient Walking Method." Data treatment simultaneously.
- Approximation / Desirability Function calculates distance from target = "Survival Function."
- Finally selects Solution

> Output:

Recipe with Ingredients and its Properties

Starting Points:

Wherever cluster of Data can be Identified which shortens the distance to one of the targets





ML: Recurrent Al Program



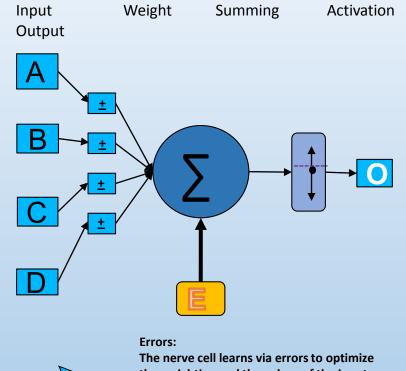
Source: S. Velasco in Spektrum 11/21

Challenges and Hints to Machine Learning [ML] with "Back Propagation" in rubber compounding:

- Time consuming testing specifically long term aging / dynamic
- Compound preparation to generate data with high effort.

(Tests with data generated in the laboratory failed in the past)

- Database standardization
 - **o** Basic data collective
 - Specific data collective
- Identification of data errors
 - **o** Errors, if Data transferred
 - Compound preparation / measurement errors



the weighting and the values of the input function.

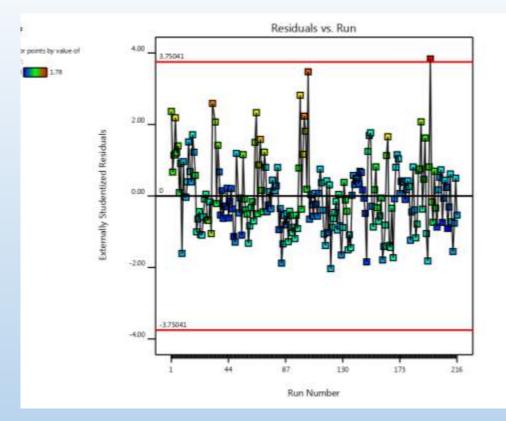
ML: Recurrent Al Program



How Neuronal Nets learn?

The weight functions between knots is adjusted through:

- Training with the difference between calculated and true value
- > This difference (error) is not obvious
 - **o** Fitting to the dimension of the value
 - **The error must be a number** Each Property needs another error number assigned
- Machine Learning: Error must be constant, but not subject to fluctuation or variation



Diagnostics of Hardening Factor

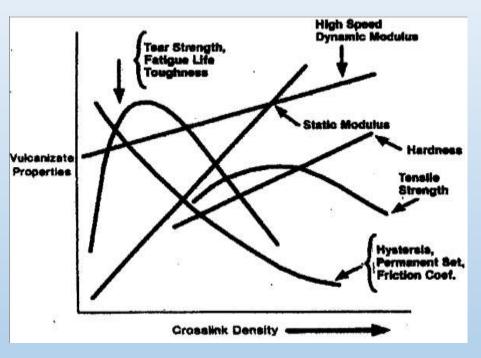
Feed Forward Al How to improve Dataset

Prediction of Compound inside 95% Confidence Interval

Elimination of Outliers

- Correlation analysis of Properties
- Properties correlated to Crosslink Density
- Properties correlated among themselves by nature

Correlation between crosslink density and physical properties



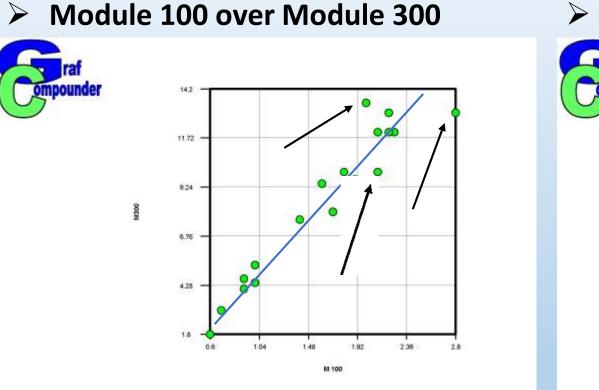
Source: D. Hertz, Elastomerics 1984, A.Y. Coran, in Science Technology of Rubber, § Vulcanization, Academic Press 1994



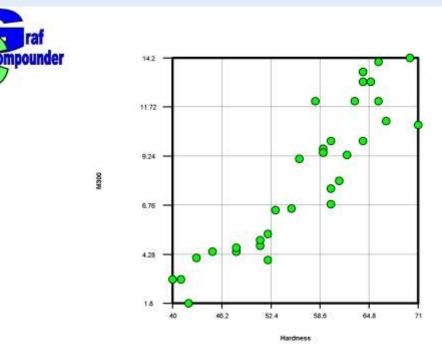


Correlation in Incidental Database

Source: NR-Data MRPRA



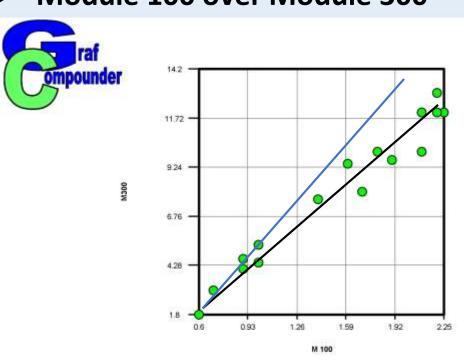
Hardness over Module 300





Correlation in Incidental Database

Source: NR-Data MRPRA



Module 100 over Module 300

- Cleaning the Data
- Inactivation of Datasets, which large
 - distance from regression line
 - $\,\circ\,$ Mouse click right
 - \odot Click on Refresh recipes
 - **Observe shift in regression line**



Spread of Data in Incidental Database

Frequency Distribution of Ingredients

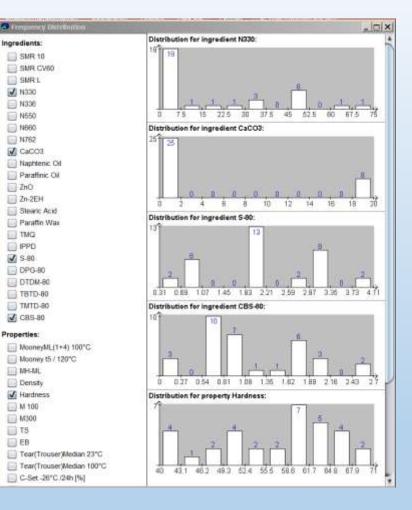
Distribution of Properties

Standardization of Properties:

• Testing according Specification (ISO, ASTM)

Additional Testing Procedures (OEM)

Documentation Standards



TS I EB

Experimentation: Decrease of Variation, Increase Precision

Laboratory Mixing Machine: Variation

 \circ Raw Material / Process Protocol Influences

➤Testing

- \odot Test Protocol: 5 instead of 3 samples per Test
- **o** Evaluation of Measurement Error

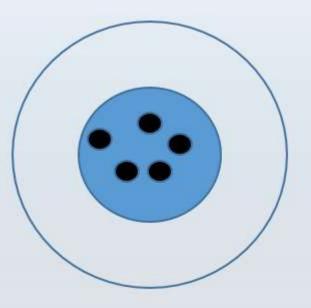
(Man – Machine – Material)

 \odot Design of Experiments: Number of Repeats

> Round Robin Testing with external Laboratories



Source: C.E. McCormick, Evaluating and Utilizing the Precision of a Test Method; Elastomerics 1983



Good Accuracy Good Precision



Prediction and Repeat of Experiments in the Laboratory

	EPM Compo	und No1	
	Predicted	Test results	Deviation
Hardness	69.99	70.00	0.01%
Tensile at Break	19.56	18.75	2.16%
Elongation at Break	338.61	339.00	0.06%
M 100	3.87	4.75	9.26%
C-Set 23°C / 22h	10.28	10.91	2.89%

EPM Compound No2

Predicted	Test results	Deviation
60.28	61.00	0.59%
15.74	18.08	6.47%
513.48	476.00	3.94%
2.04	3.05	16.56%
10.00	9.97	0.15%

Data in good agreement except Modulus 100



Feed Forward AI: What is the advantage?

Compound Prediction is possible with any data set Data set can be small or large

All significant parameters should be included in the query simultaneously

- 2-3 Properties in the query makes no sense.
- Most specification values, but at tighter limits
 - Improve query with "Weights" and "Trdoff"

Criteria:							Criteria:			Output:	
Name	Min	Max	From	То	Weight	Trdoff	Name	Min	Max F		1
ZnO	1.2	4									<u> </u>
TMQ	0	1.2					Polymer 1	0	115		
BDMA/S	0	1.1					Polymer 2	0	0		5
TAC-50	0	1.4					Polymer 3	0	100		<
S- 80	0	0.3					Polymer 4	0	0	1	
Oil	0	50					Polymer 5	0	0		
CB 02	0	78					Polymer 6M	0	50		
CB 01	0	95					Stearic Acid	0.4	0.4	0.4	
Filler 01	0	30					Process Aid 1	0	4	3.165	
Perkadox 14/40	6	6					PEG	0	2	0.255	
							Process Aid 2	0	4	0.8775	
Density	1.082	1.17					MgO	0	4	2.069	
Hardness	53	79.5		70			ZnO	1.2	4	3.2	
Tensile Strength	13.65	22.8					TMQ	0	1.2	1.2	
Elongation at	247	605					BDMA/S	0	1.1	0.85975	
M100	1.28	6.24					TAC-50	0	1.4	0.3135	
M300	5.05	16.58					S- 80	0	0.3	0.06475	
CSET-22h/23C	7.41	14.55		9	20		Oil	0	50	11.8875	
CSET-22h/150C	9.8	32.38		25			CB 02	0	78	58.8125	
Delta H	1	9	-5	3	10		CB 01	0	95	19.85	
Delta TS	-13.21	31.14	-5	10			Filler 01	0	30	1.9125	
Delta EB	-14.74	18.62	0	8	50		Perkadox 14/40	6	6	6	
Delta M100	-9.17	65.68	-5	8	20						
Delta M300	-8.13	18.94					Density	1.082	1.17	1.117973	
Low Temp	-59.09	49.9		-50	10		Hardness	53	79.5	70.9475	
Tear	3.92	12.44					Tensile Strength	13.65	22.8	19.31475	
							Elengation at	247	EUE	_000 AE7E	

AI: Conclusion

Feed Forward AI: GRAFCOMPOUNDER

- Compound History
- > Analyze
- Simulate
- > Select
- Confirm



- > Explore Materials
- > Evaluate
- > Decide
- Conclude
- > Confirm



Conclusion



Feed Forward AI: Compounder Program

- Compound Cost target included
- Starting Formula for Compound Development
- Simulation of Recipe for Specification Adjustments
- Historic Data usage and improved Data storage in GC Format

Statistic Experimental Design

- Evaluation of New Materials
- Cost optimization in Compounding
- Design / Improvement of New Processes
- Process Window to Control Quality according SPC

Preferred Rubber Compound Development Strategy: Combination of Compound Simulation from Database with Statistic Experimental Design Experimentation Procedure

Both methods have their justification.



Thank you for joining this presentation.

→Questions, Remarks, Discussion?



More information under: www.grafcompounder.com