Artificial Intelligence and Other Digitalization Techniques for the Material Science Industry

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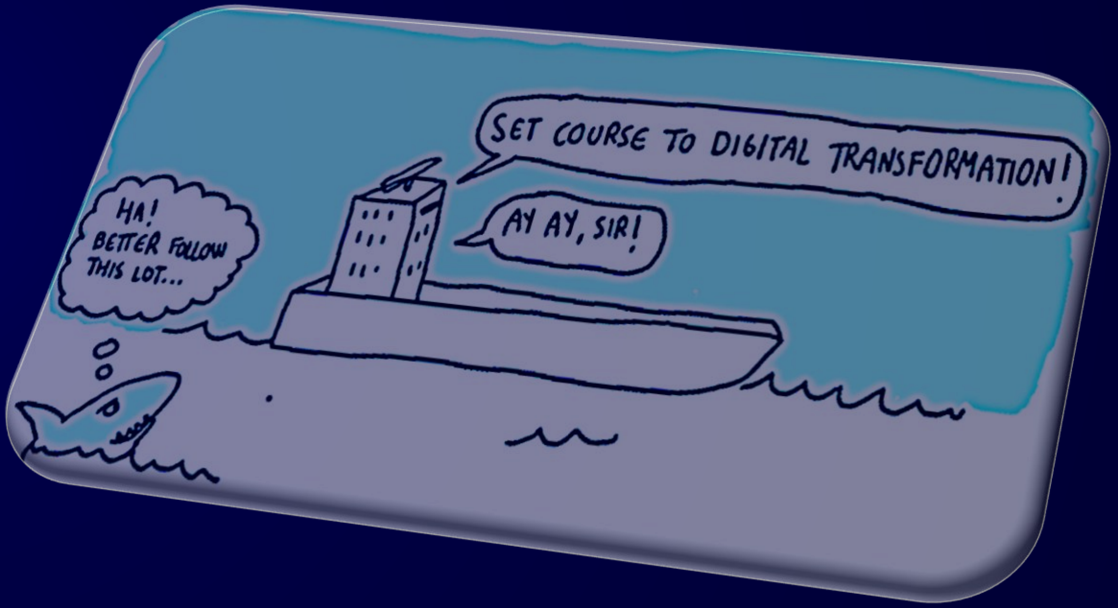
Senior Fellow



https://www.businessillustrator.com/what-is-digital-transformation-cartoon-infographic/

Intugent

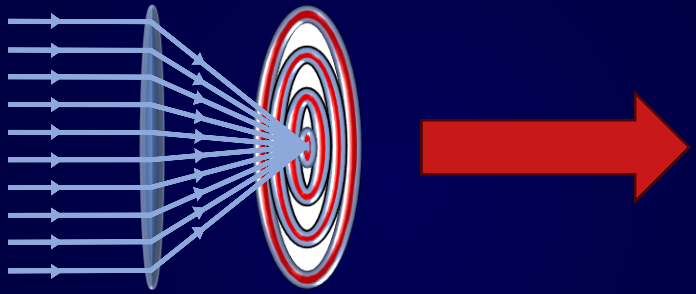
The scientific Artificial Intelligence & Digitalization Company

Intugent

The scientific Artificial Intelligence & Digitalization Company

Core Capabilities

- Scientific Artificial Intelligence (sAI)
- Material Science
- Process Simulation
- Data Sciences
- Information Technology



Value Creation

- Reduced developmental costs & times
- Success at the 1st commercial trial
- Higher quality innovations
- New application domains
- Simpler Digital Work Process (DWP)

Intugent Edge

Proven Track Record

Commercialized (DWP) for multi-billion $ companies

Excellent User Experience

Users do not need any background in AI or Math Modelling

scientific Artificial Intelligence

Pioneered sAI. Combines science and AI. High powered computers are not needed

Superb User Support

Each DWP is tailored to client's process. In house SME's in all core capabilities

Grand Challenges to Composite Growth

- Development of a Sufficiently Skilled Workforce
- Reduction of Developmental & Cycle Times
- Expansion of Knowledge and Tools (Modeling, …)
- Advancement of the Performance Materials

Original designed by Freepick.com

* (FIBERS Consortium Study 2019, Funded by NIST)

Predictive Models, Intuition and Gut Feeling

- Rational / Mathematical Analysis
  - Require long times to obtain predictions
- Intuition / Gut Feeling
  - Near instantaneous subconscious processing
  - Rooted in years of personal experience, knowhow, and imagination

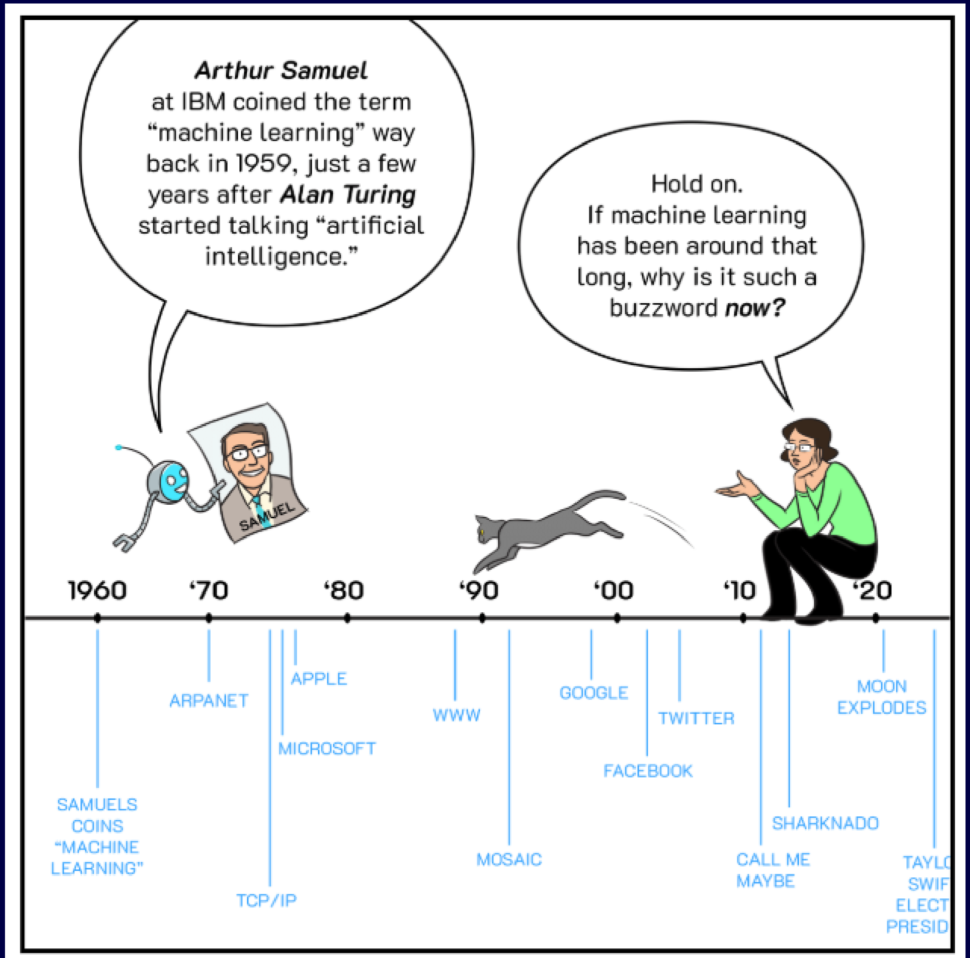
Original designed by Freepick.com

Overview

1. Introduction to Digital Transformation and Artificial Intelligence
2. Neural Networks – Development and Applications
3. Case Studies
4. Other Digitalization Techniques (Scaleup Models

Part 1

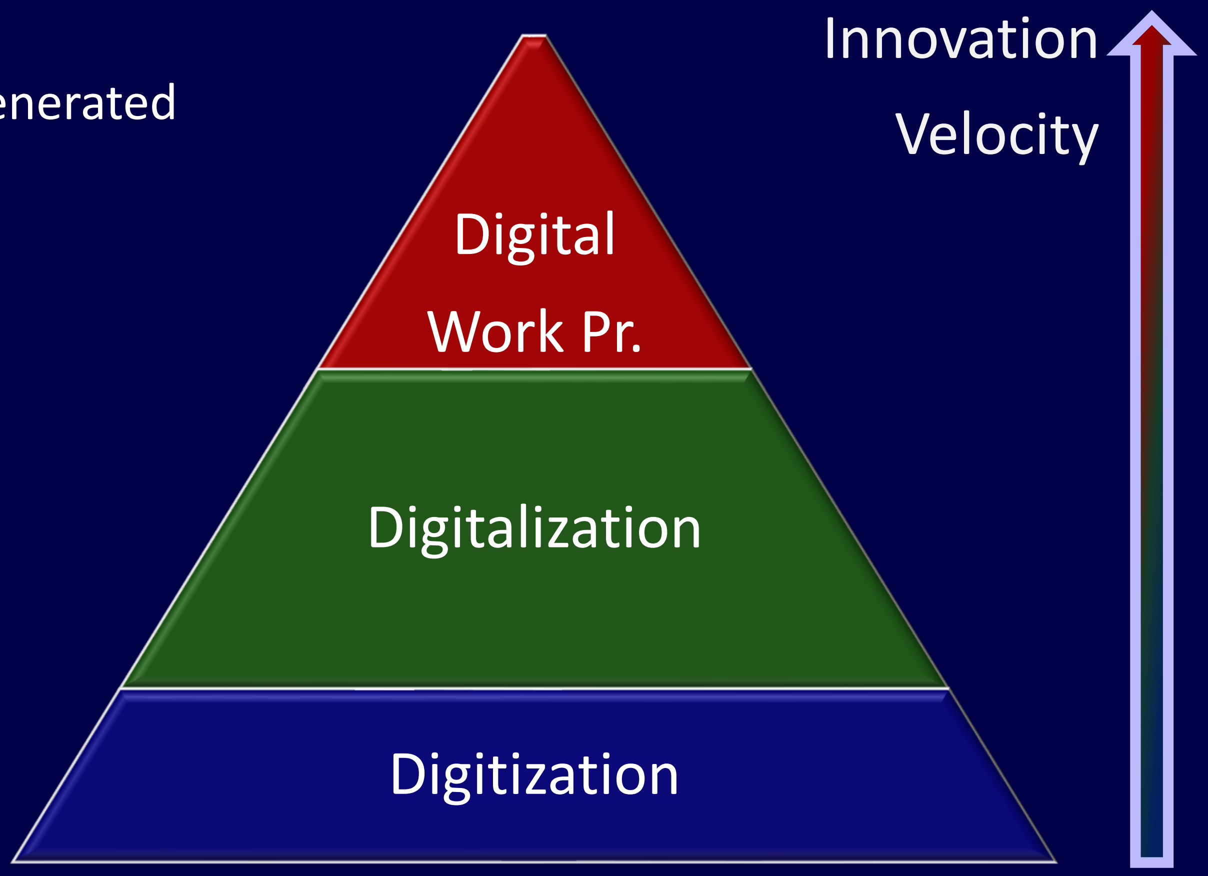
Introduction to Digital Transformation & Artificial Intelligence



https://cloud.google.com/products/ai/ml-comic-1

Digitalization and Digital Work Process

- Digitization
  - Collection of data in digital form as it is being generated
- Digitalization
  - Artificial Intelligence
  - Science based math models
  - Process simulation
  - Databases and Visualization
- Digital Work Process
  - Intuitive, user experience
  - Shorten the work process



Digital Transformation:- Development and Implementation

1. Digital Work Process

- Based on the existing work process
- Collect data as it is being generated

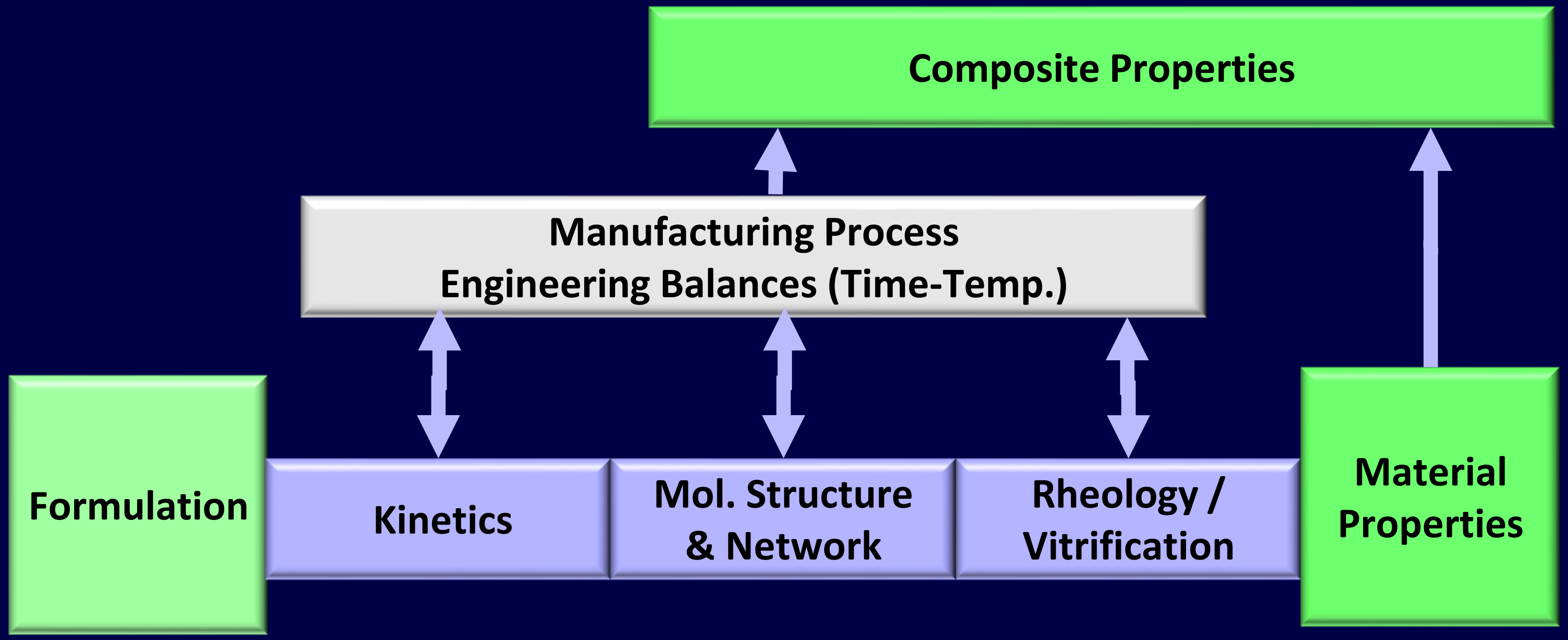
2. Digitalization: Low Hanging Fruits

- Collect data as it is being generated
- Available Statistical and Math models for predicting properties
- Process simulation models
- Groundwork for AI/sAI models

3. Digitalization (AI/sAI)

- Collect data as it is being generated
- Develop AI/sAI models
- Use AI/sAI models in predictive mode (virtual lab)
- Prescriptive mode or reverse engineering is optional

Materials Paradigm / Process Domain



Property Prediction Models

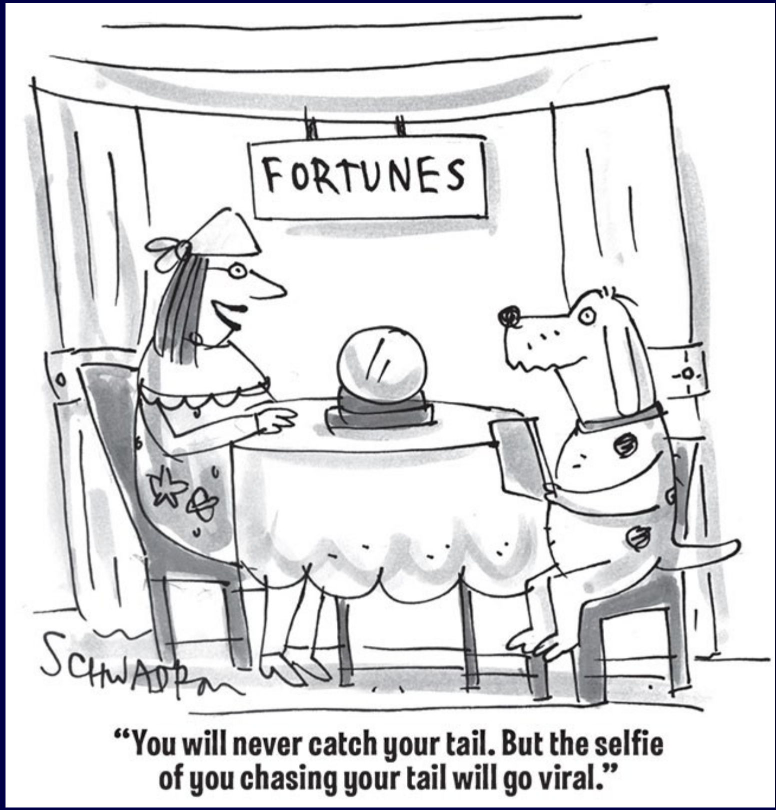
- Predict properties after reactions are complete (lab or commercial scale)
- AI & Math Models

Process Simulation Models

- Can we complete processes under commercial application conditions
- Rheokinetic scaleup models

Predictive Models

- Statistical Models
- Scientific Math Models
  - Scaleup Models
- Artificial Intelligence Models
- Scientific Artificial Intelligence Models



Comic by Harley Schwadron
https://jokes.scoutlife.org/topics/fortune-teller-jokes/

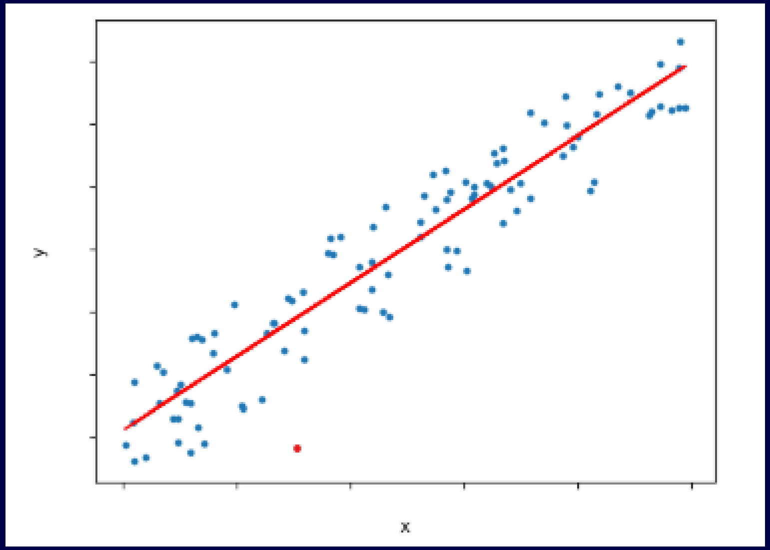
Statistical Models

- Linear Regression

$$\hat{Y} = m\,X + C$$

  - m and C are obtained by minimizing

$$\mathrm{SSE} = \mathrm{E} \;= \sum(\hat{y} \; - y)^2$$



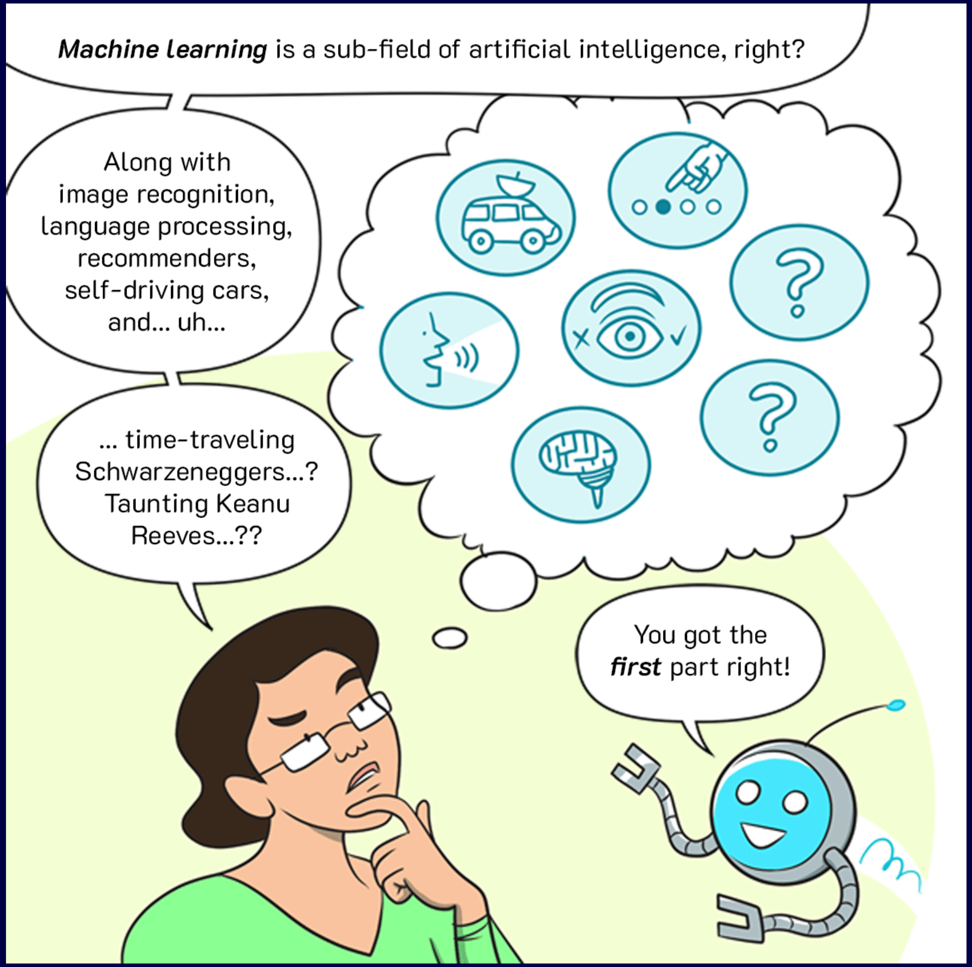
https://algogene.com/community/post/111

- Multiple Linear Regression

$$\hat{Y} = c_o + c_1\,X_1 + c_2\,X_2 + c_3\,X_3 + \cdots$$

More on Regression later

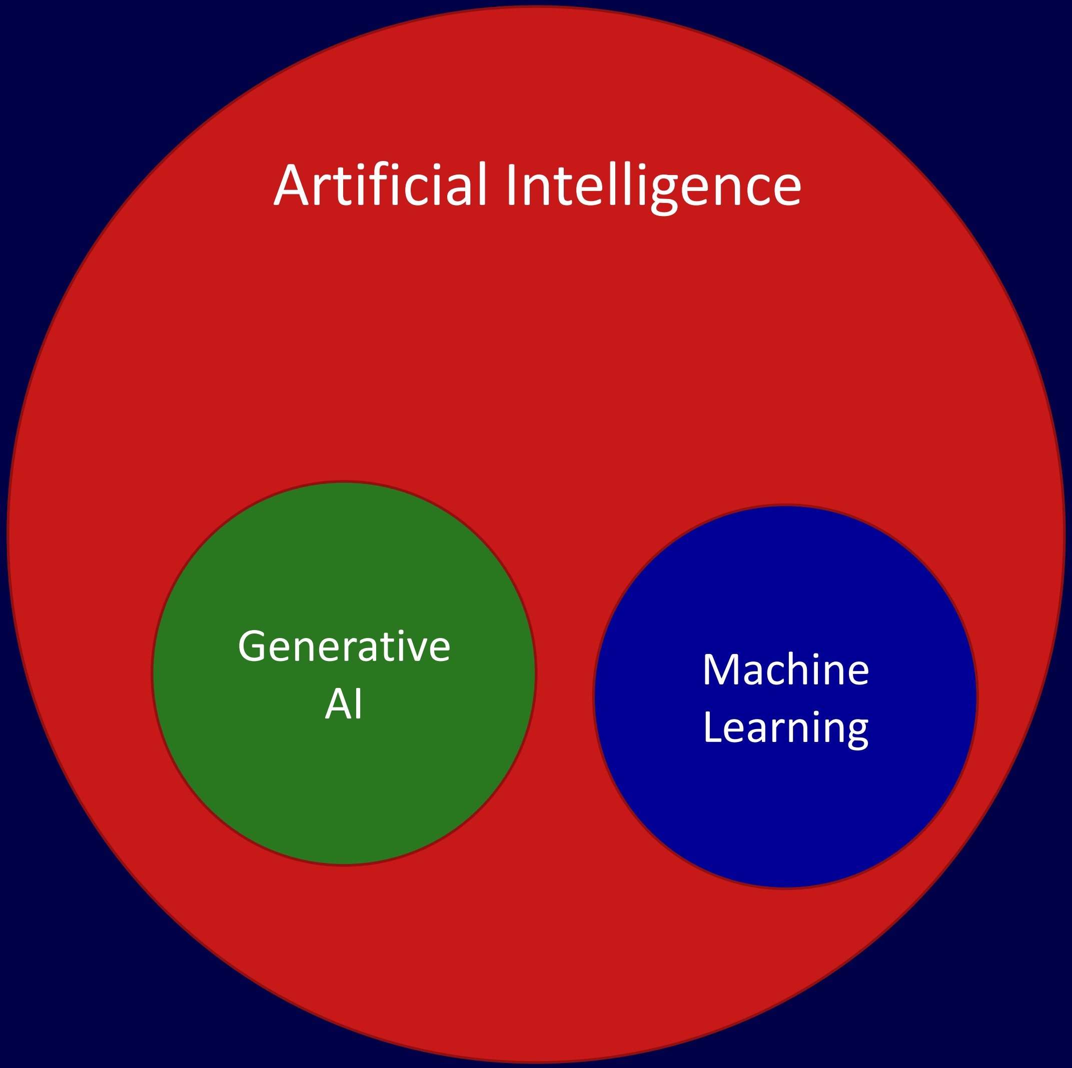
Artificial Intelligence
&
Machine Learning



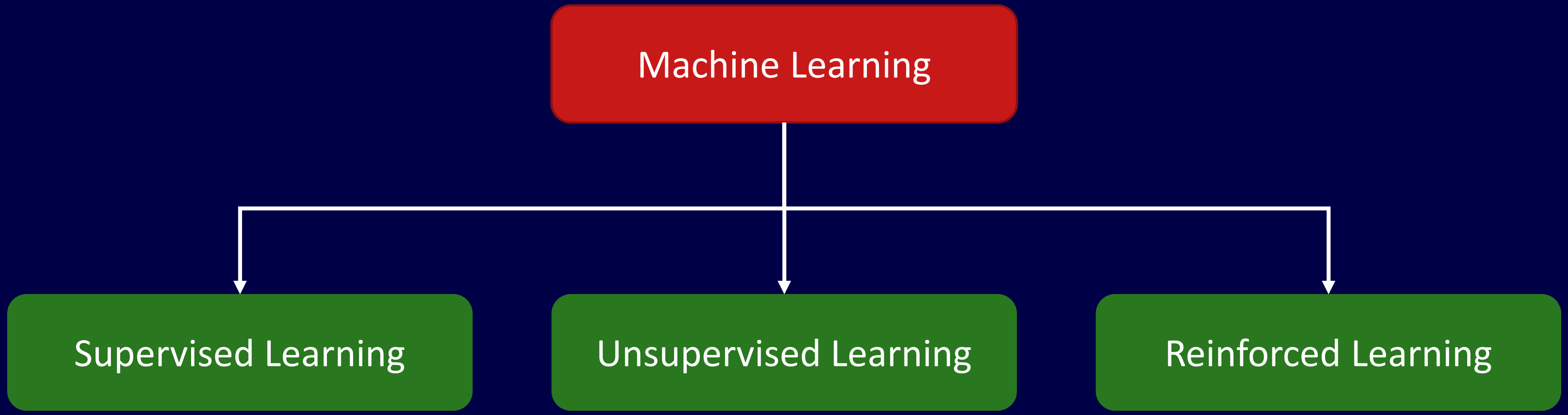
https://cloud.google.com/products/ai/ml-comic-1

Artificial Intelligence & Machine Learning

- Artificial Intelligence
  - Simulation of human intelligence
- Generative AI
  - Generate new content
  - ChatGPT, Copilot, DeepSeek, Dall-E
  - AI agents such as Alexa, Gemini, …
- Machine Learning
  - Development of algorithms/computer programs capable of learning from data and making predictions

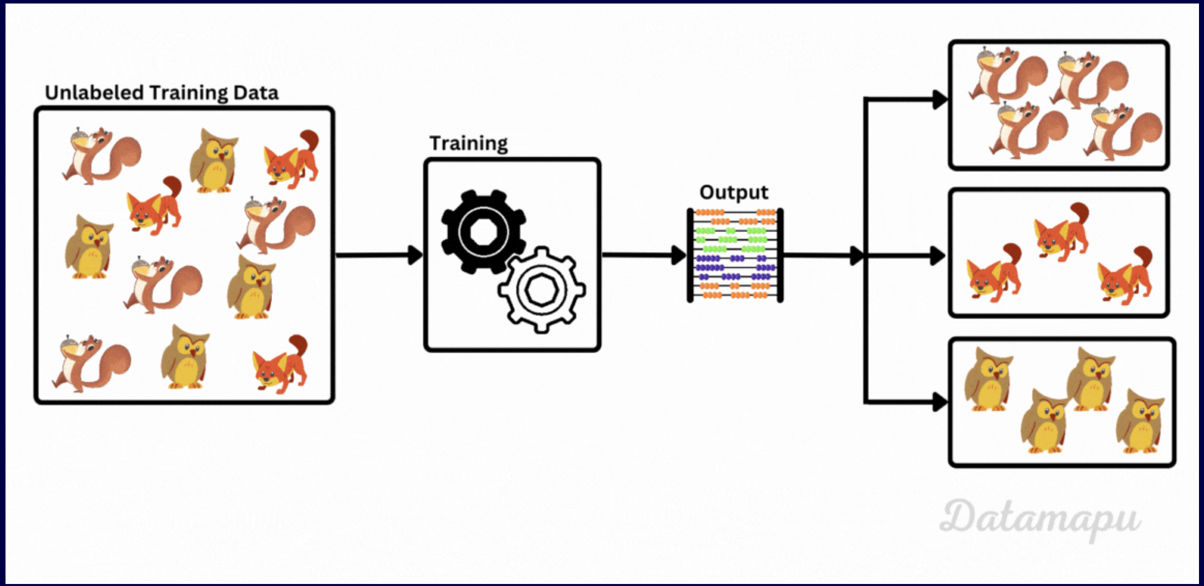


Type of Machine Learning



Machine Learning – Unsupervised Learning

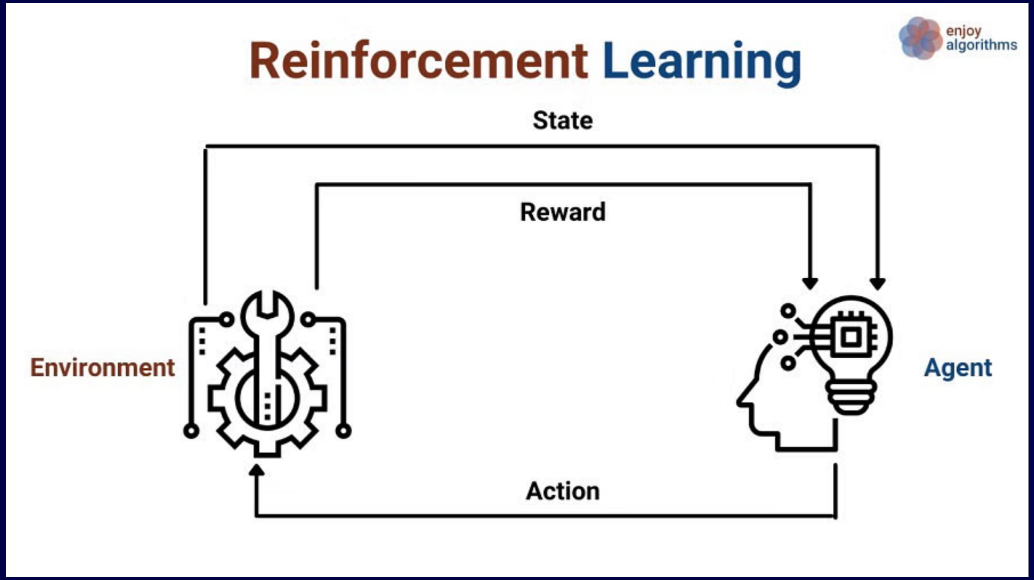
- How does it work
  - The datapoint does not contain any label or output value
  - The model identifies pattern or grouping
  - Abnormal patterns are identified
- Applications
  - Customer segmentation
  - Anomaly detection
  - Cyber security



https://datamapu.com/posts/ml_concepts/supervised_unsupervised/

Machine Learning – Reinforced Learning

- How does it work
  - An agent or robot is programmed to perform a task
  - Feedback from environment provides reinforcement
  - +ve reinforcement increase the frequency of the behavior
  - -ve reinforcement decrease the frequency of the behavior
- Applications
  - Robotics
  - Self-driving Automobiles
  - Video Games

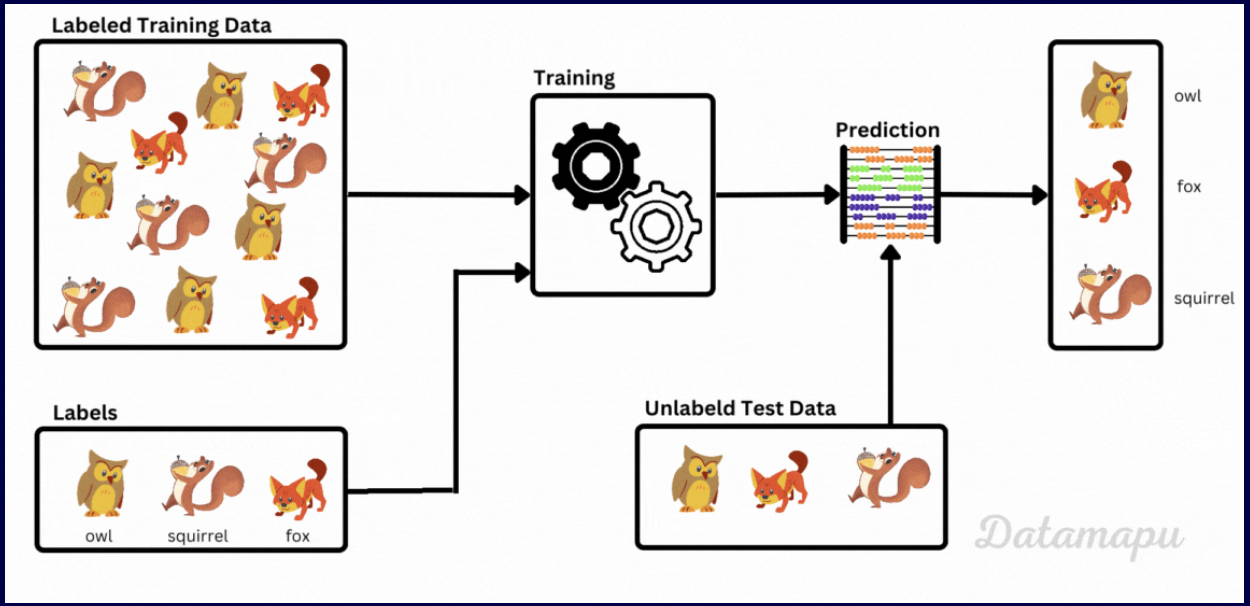


https://www.projectpro.io/article/types-of-machine-learning/623

Machine Learning – Supervised Learning

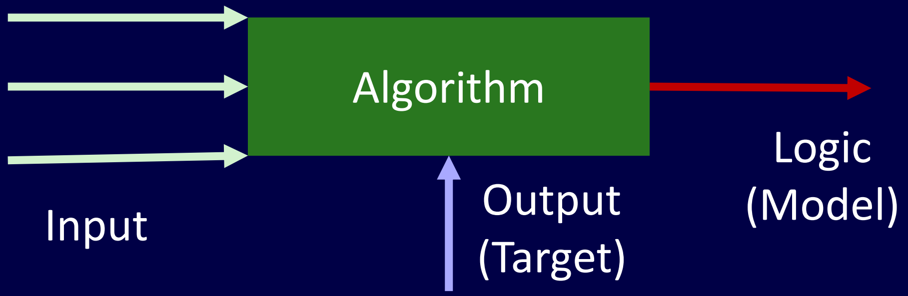
- How does it work
  - A datapoint contains input data and output (label, target) value
  - A known dataset is used to learn relationship between input and output
  - Model is then used to predict output given the input

- Applications
  - Image classification
  - Medical diagnosis
  - Speech recognition
  - Predicting continuous values such as stock prices, house prices, and **material properties**

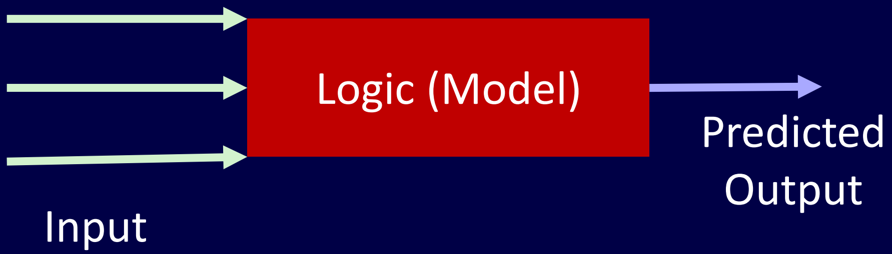


https://datamapu.com/posts/ml_concepts/supervised_unsupervised/

Supervised Machine Learning

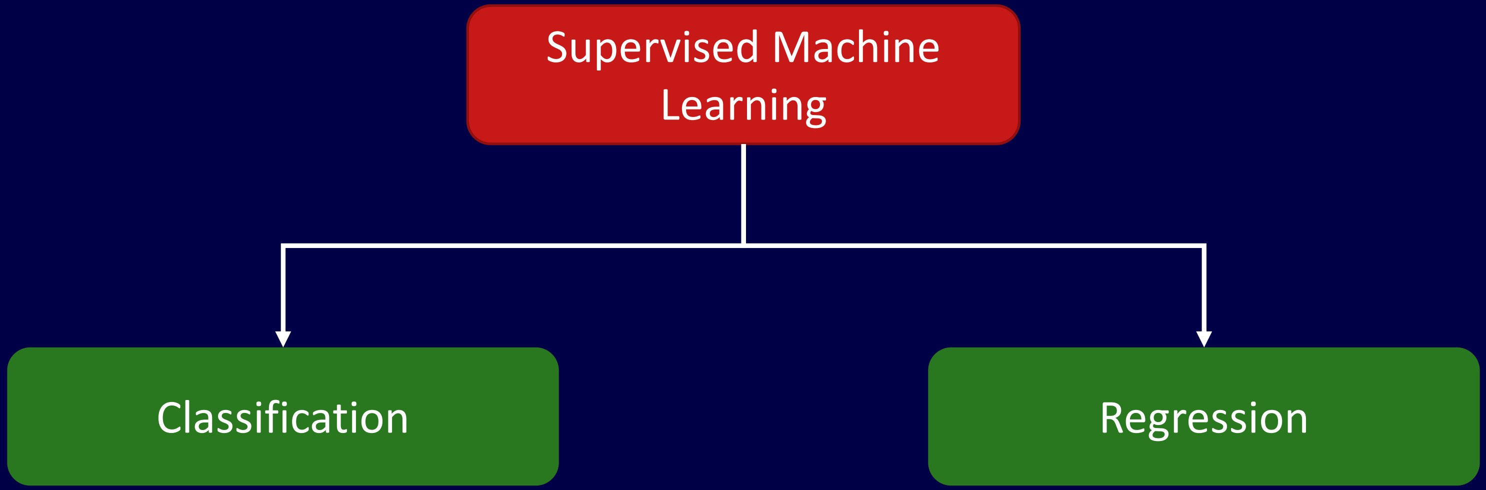


Training / Learning



Prediction

Types of Supervised Machine Learning



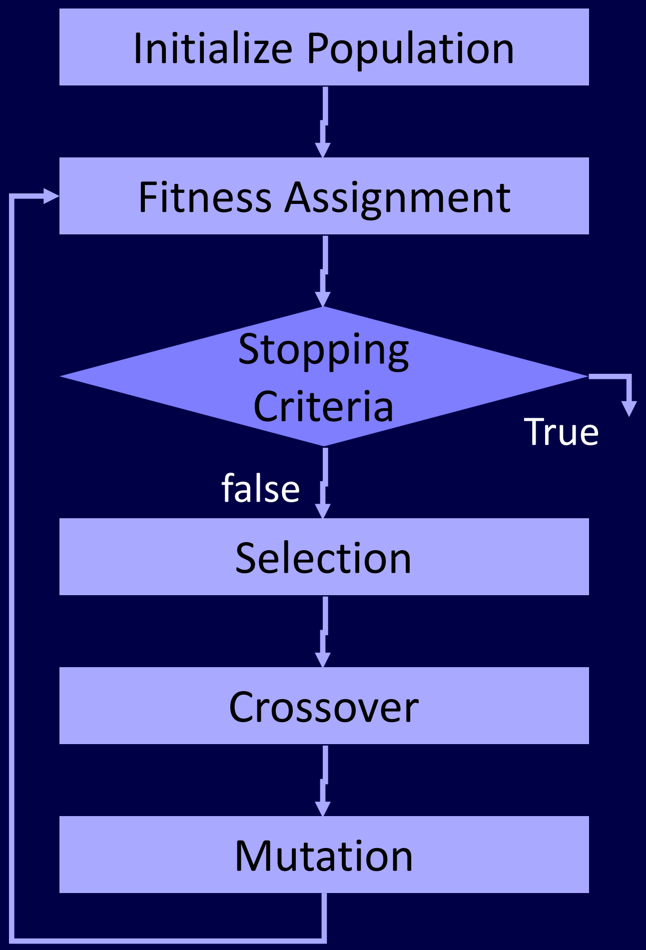
- Output is discrete or categorical
- Examples
  - Spam/no spam,
  - Image classification
  - Diagnostics

- Output is Continuous
- Examples
  - Risk assessment,
  - Stock market
  - **Material properties**

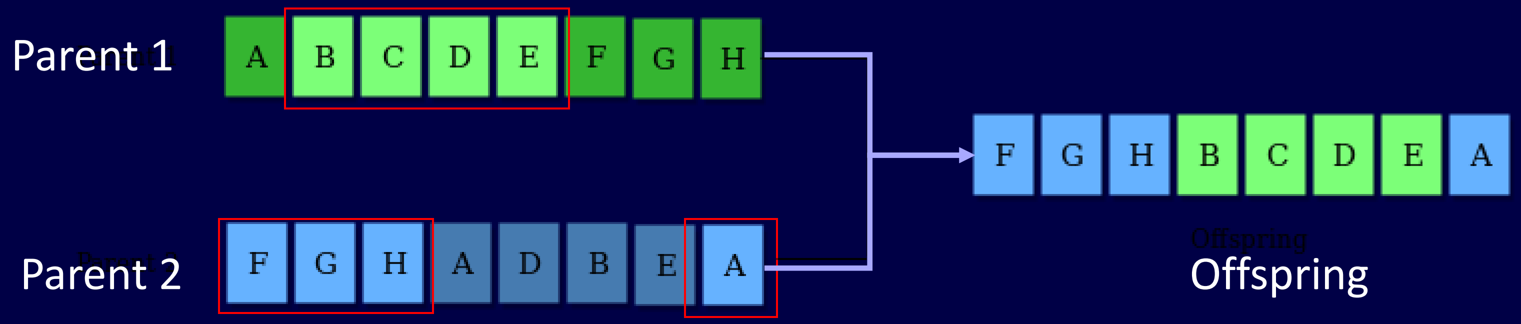
Supervised Learning: Regression

- Artificial neural networks
- Decision Tree
- Random Forest Ensemble
- Genetic Algorithms

Genetic Algorithms



Crossover



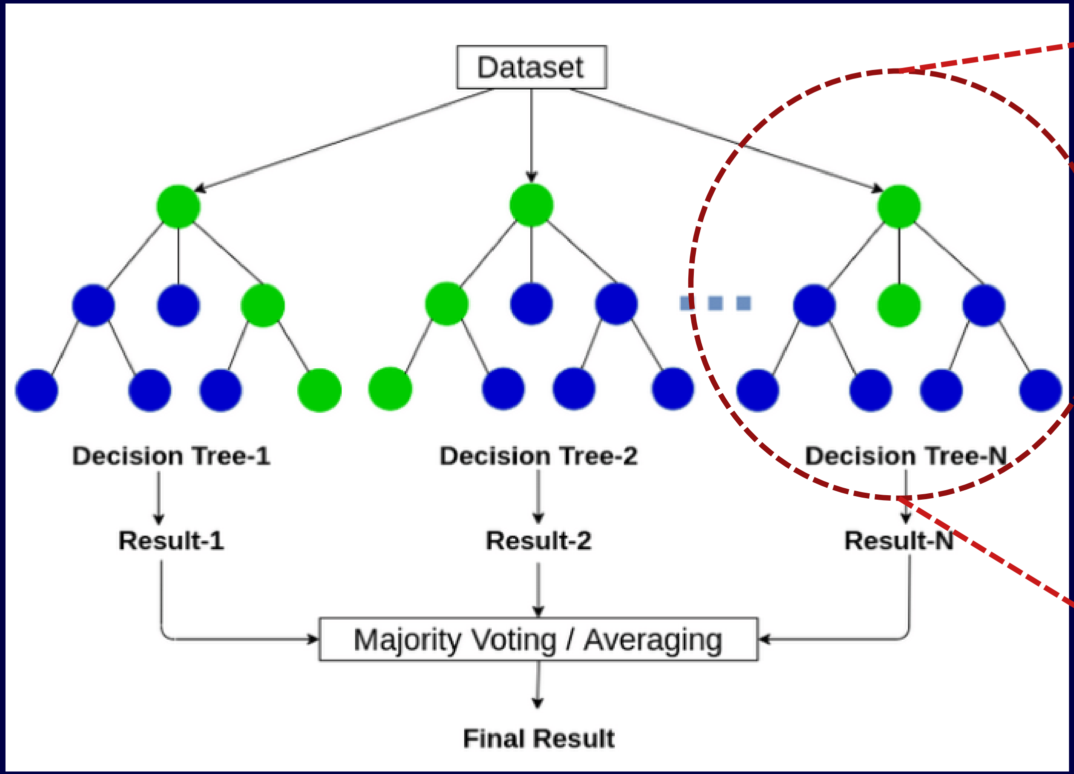
Mutation

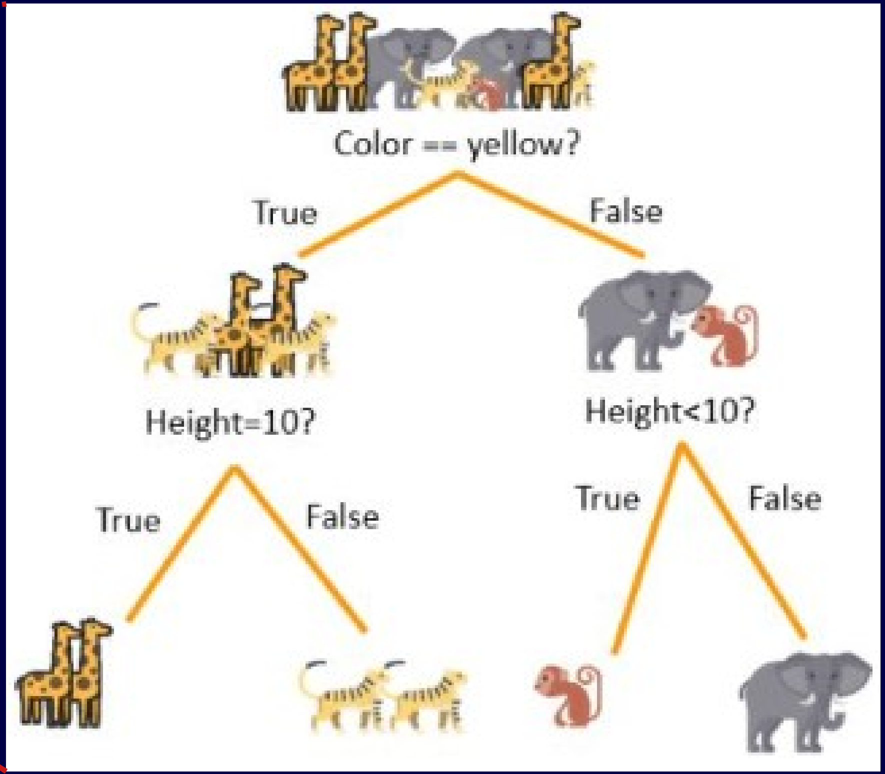
https://www.geeksforgeeks.org/genetic-algorithms/

Limited Application

- Robotics, self driving, financial modelling
- Primarily used to fine tune parameters of other machine learning methods such as neural networks

Decision Tree / Random Forest Models





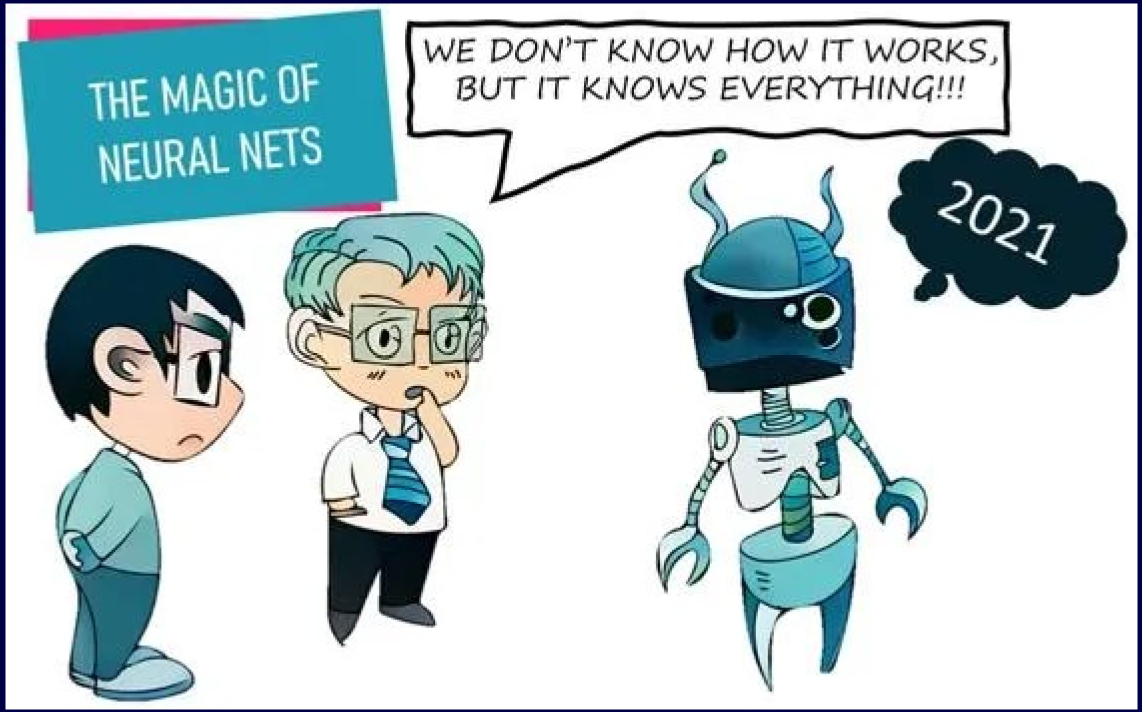
DOI:10.3390/w13040547

https://algogene.com/community/post/111

* A continuous variable being treated as discrete variable?

Part 2

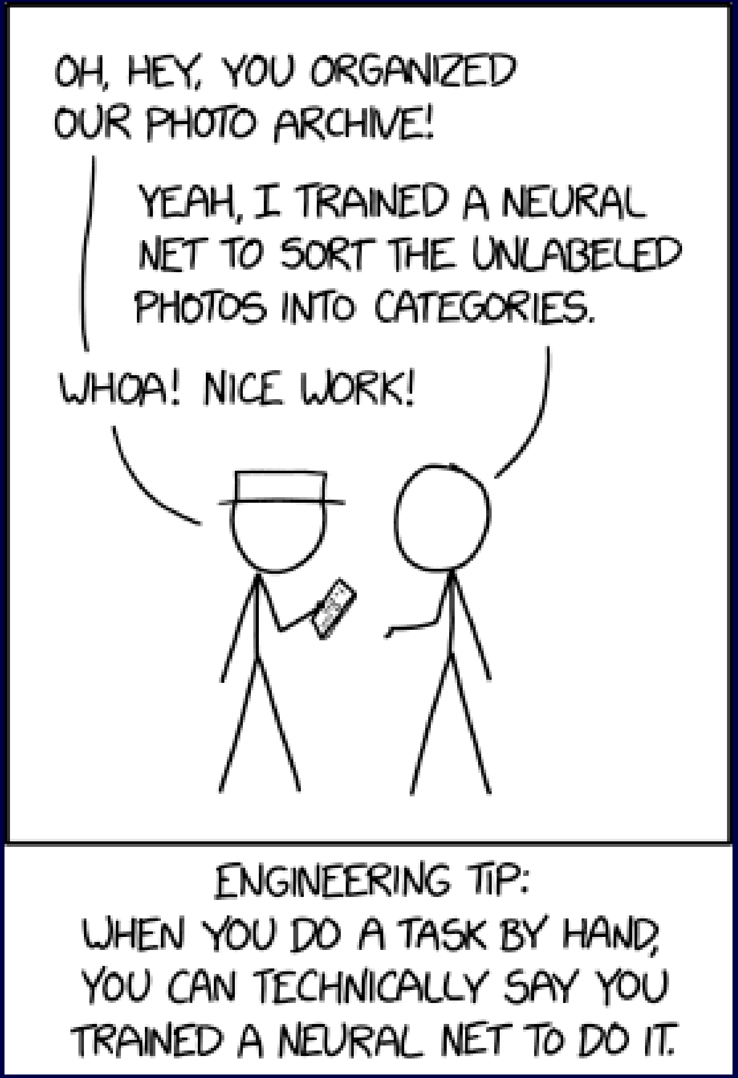
Neural Networks



https://medium.com/@priyadharshini.18nov/how-to-make-art-with-ai-and-neural-networks-42f6bb751416

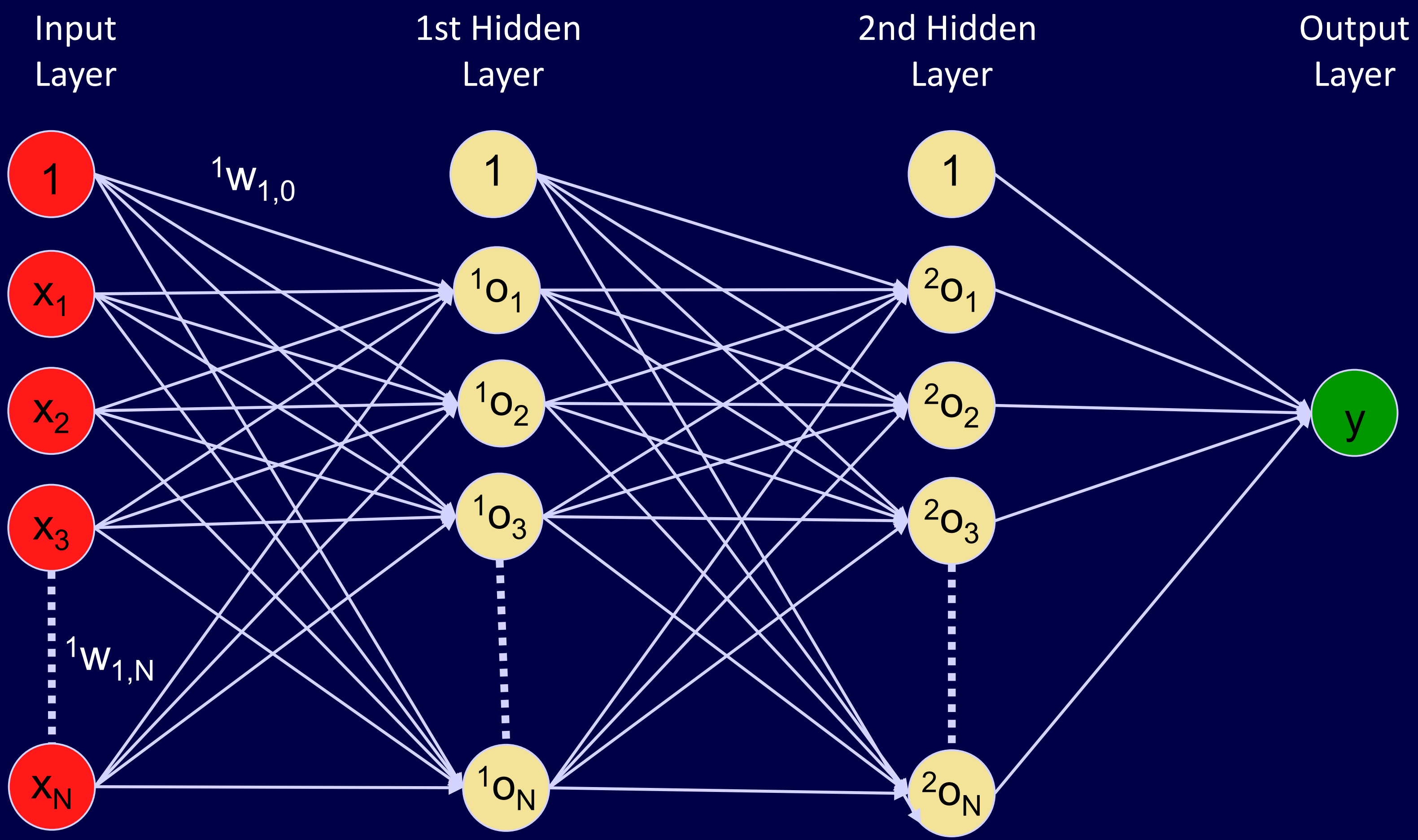
Neural Networks

- Highly robust method for approximating real value problems
- Method inspired from neurons and behavior of brain
- Very good at approximating complex functions and relationships
- Based on simple mathematical formalism
- Applications
  - Facial recognition
  - Stock market predictions
  - Material properties



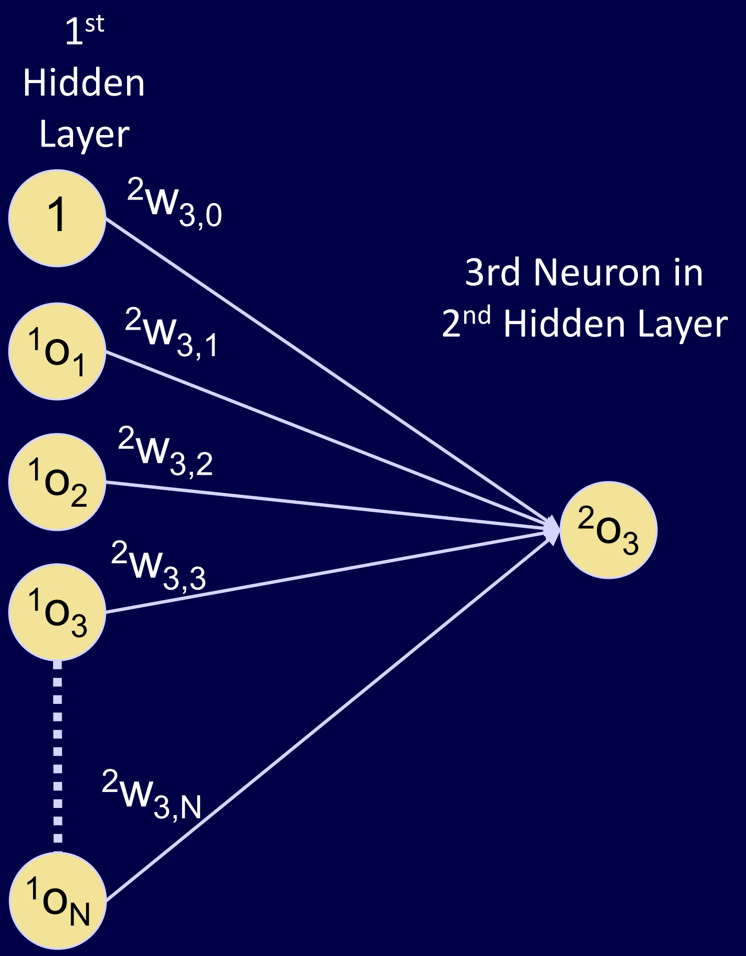
https://www.explainxkcd.com/wiki/index.php/2173:_Trained_a_Neural_Net

Neural Networks – Building Blocks



- Each dot is a neuron
- Each line represents a link (dependence), w, that is estimated during training
- Any number of hidden layers can be used
- x_1, x_2, x_3 … x_N are input variables

Neural Networks – Mathematical Formalism



- Value of a neuron (for example $^1h_1$) in a hidden layer is determined in two steps.
    1. A new variable is defined as a linear combination of the all the neurons in the previous layer
    2. New variable is transformed through an activation function to introduce nonlinear behavior

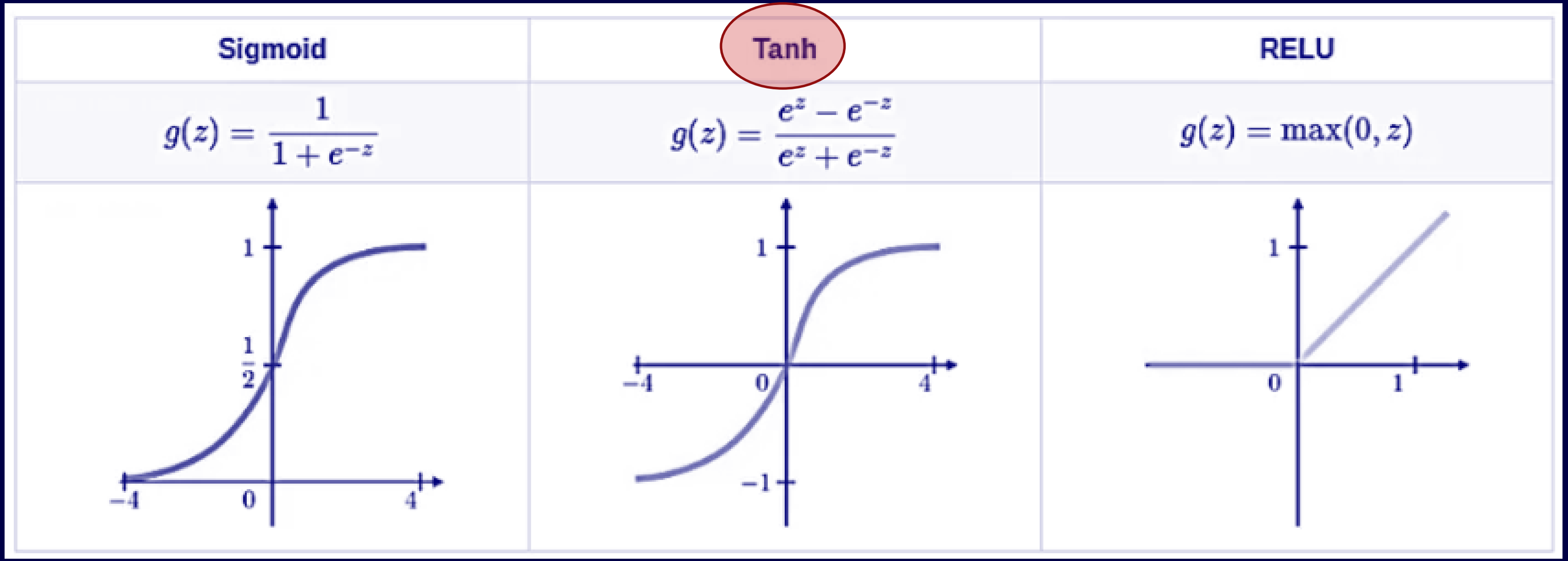
$$^2a_3 = {}^2w_{3,0} + {}^2w_{3,1}\, {}^2o_1 + {}^2w_{3,2}\, o_2 + {}^2w_{3,3}\, {}^2o_3 + \ldots + {}^2w_{3,N}\, {}^2o_N$$

$^2o_3 = g(^2a_3)$, g is the activation function

- Compare it to Multiple Linear Regression

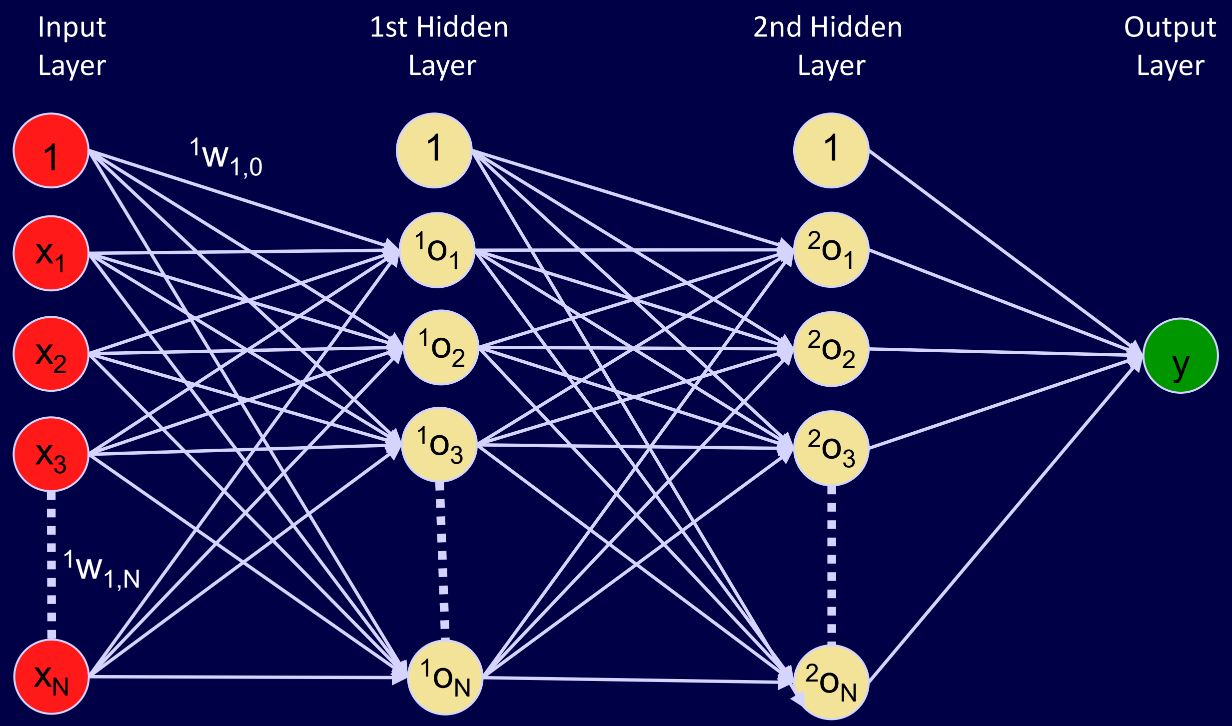
$$\hat{Y} = c_o + c_1\, X_1 + c_2\, X_2 + c_3\, X_3 + \cdots$$

Neural Networks – Activation Functions



Output Range	0 to 1	-1 to 1	0 to 1
Max. slope	0.25	1	1
Advantage	Output layer for classification problems	0 centered, converge faster	Suitable for deep learning, Computationally simple

Neural Networks – Mathematics



$$^{l}a_i = \sum_j {}^{l}w_{i,j}\ {}^{l-1}o_j$$

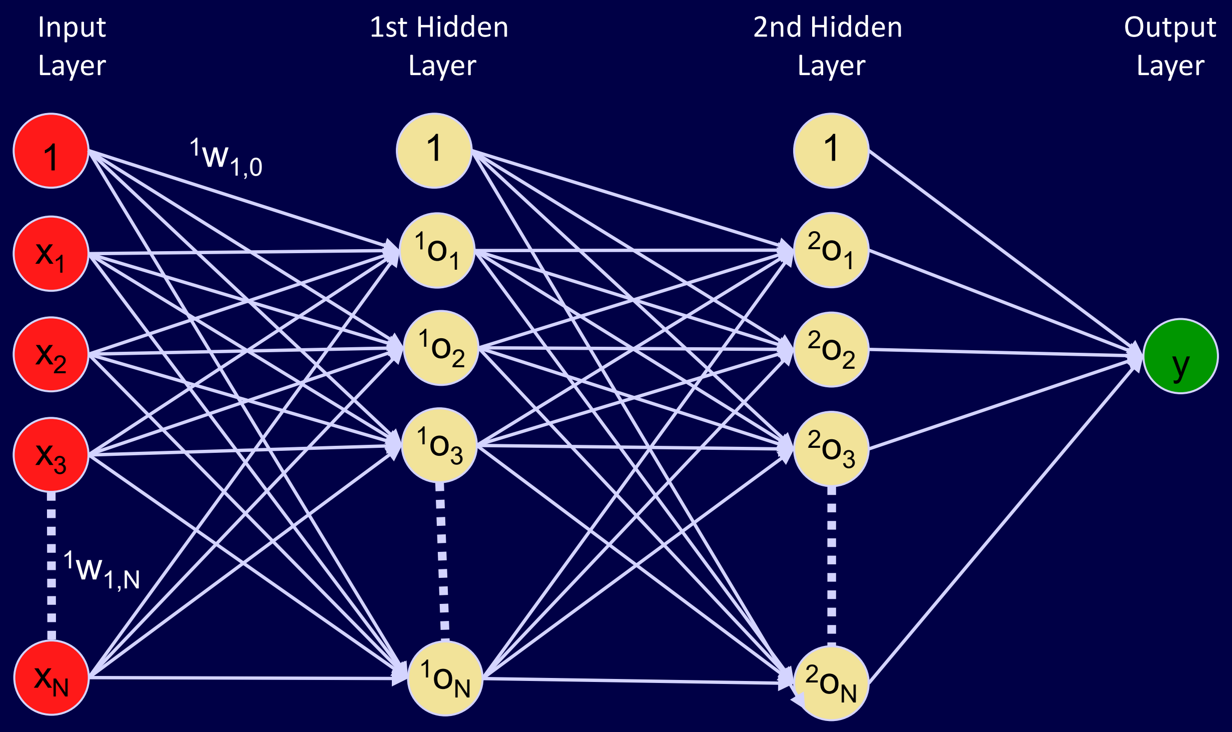
$$^{l}o_i = g\left({}^{l}a_i \right)$$

$^{l}o_i =$ value of i^{th} neuron in l^{th} layer

$^{l}w_{i,j}$ = weight used in calculations of i^{th} neuron in l^{th} layer to j^{th} neuron of previous layer

- Calculations are performed for each neuron in the hidden and the output layers
- Ws are the unknown parameters that are estimated during training of the model

Neural Networks – Mathematics



$$ {}^{l}a_i = \sum_j {}^{l}w_{i,j} \; {}^{l-1}o_j $$

$$ {}^{l}o_i = g\left({}^{l}a_i \right) $$

${}^{l}o_i =$ value of i^{th} neuron in l^{th} layer

${}^{l}w_{i,j}$ = weight used in calculations of i^{th} neuron in l^{th} layer to j^{th} neuron of previous layer

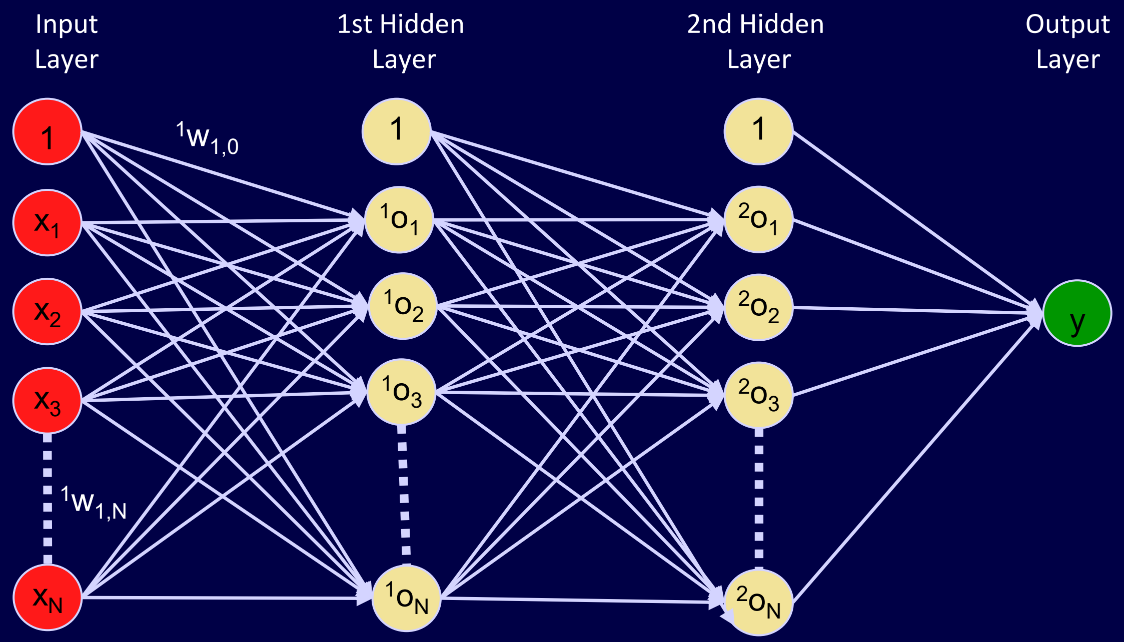
- Calculations are performed for each neuron in the hidden and the output layers.
- Ws are the unknown parameters that are estimated during training of the model

Neural Networks – Model Training

- Root Mean Square is most commonly used as measure of error or loss in estimating the values of y

$$E = \frac{1}{2\ N_d}\sum_i (\hat{y}_i\ -\ y_i)^2$$

- Object is to find values of Ws that minimize the error (loss)
- Ws are the unknown parameters that are estimated during training of the model



$$\#\ of\ Ws = \sum_l {}^{l}N\ \left({}^{l-1}N + 1\right)$$

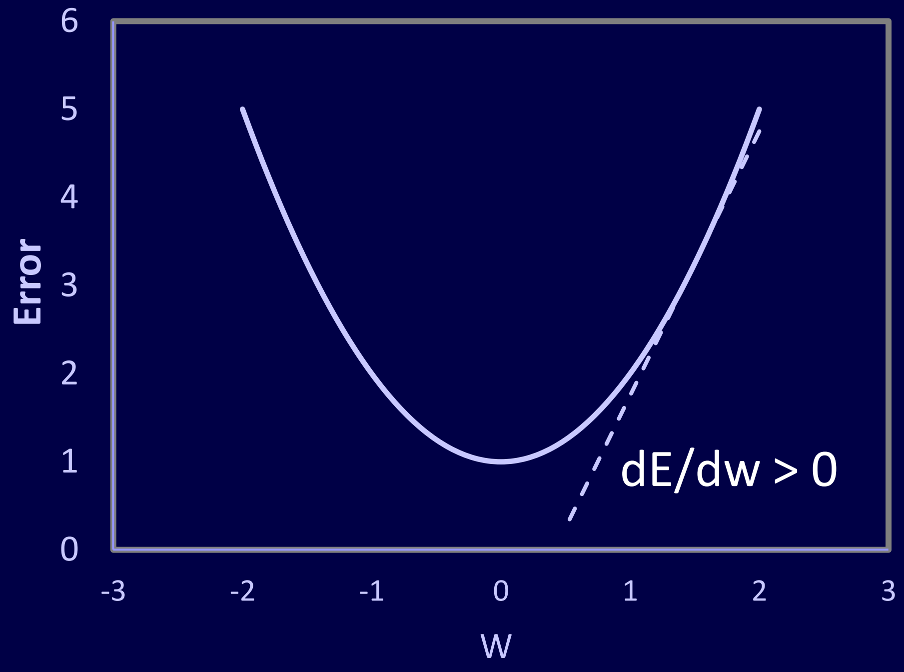
${}^{l}N$ is # of neurons in Layer ℓ

Neural Networks – Gradient Descent

- Change Ws in direction opposite to gradient

$$\Delta w = -\,\alpha \,\frac{dE}{dw}$$

- α is chosen to make a desired step change
  - A very small α may increase # of iterations to get to the solution
  - A very large α may result into oscillations and solution will not converge



- Calculations of ws and setting value of α are the most critical steps in model training solution

Neural Networks – Back Propagation

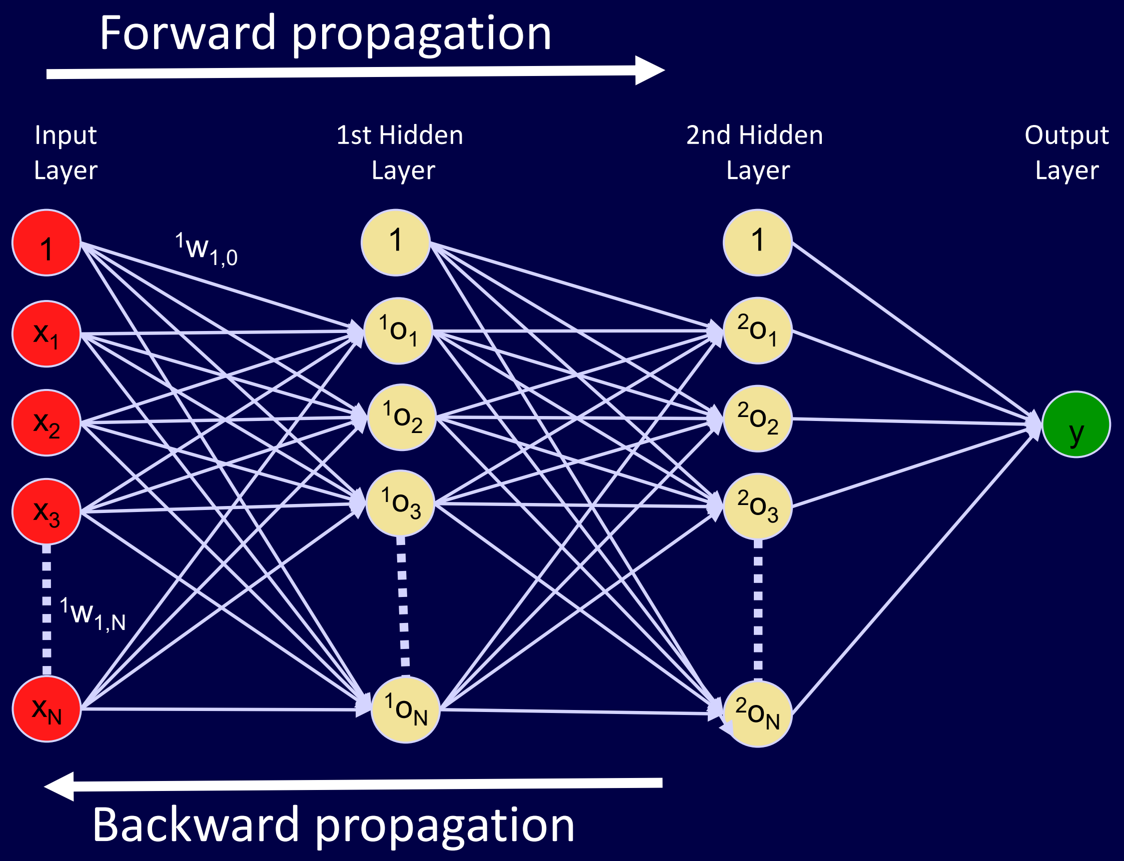
- Forward propagation calculates the value for each neuron, output and error for every data point

$$ {}^{l}a_i = \sum_j {}^{l}w_{i,j}\; {}^{l-1}o_j \qquad {}^{l}o_i = g({}^{l}a_i) $$

$$ E = \frac{1}{2\,N_d}\sum_p \left(\hat{y}_p - y_p\right)^2 $$

- Backward propagation calculates derivative of error function for each data point to optimize sets of ws

$$ \frac{\partial E}{\partial\, {}^{l}w_{i,j}} = \frac{dg}{d\,{}^{l}a_i}\; {}^{l-1}o_j \sum_j {}^{l+1}w_{i,j} \frac{\partial E}{\partial\, {}^{l+1}a_i} $$



Problem of Overfitting in Scientific Applications

https://livebook.manning.com/book/grokking-machine-learning/chapter-4/

Dr. Allen Genevera of Rice University says flawed machine learning is producing a "crisis in science“

P. Gosh, [https://www.bbc.com/news/science-environment-47267081, 16 Feb. 2019]

“Often these studies are not found out to be inaccurate until there's another real big dataset that someone applies these techniques to and says ‘oh my goodness, the results of these two studies don't overlap‘," she said.

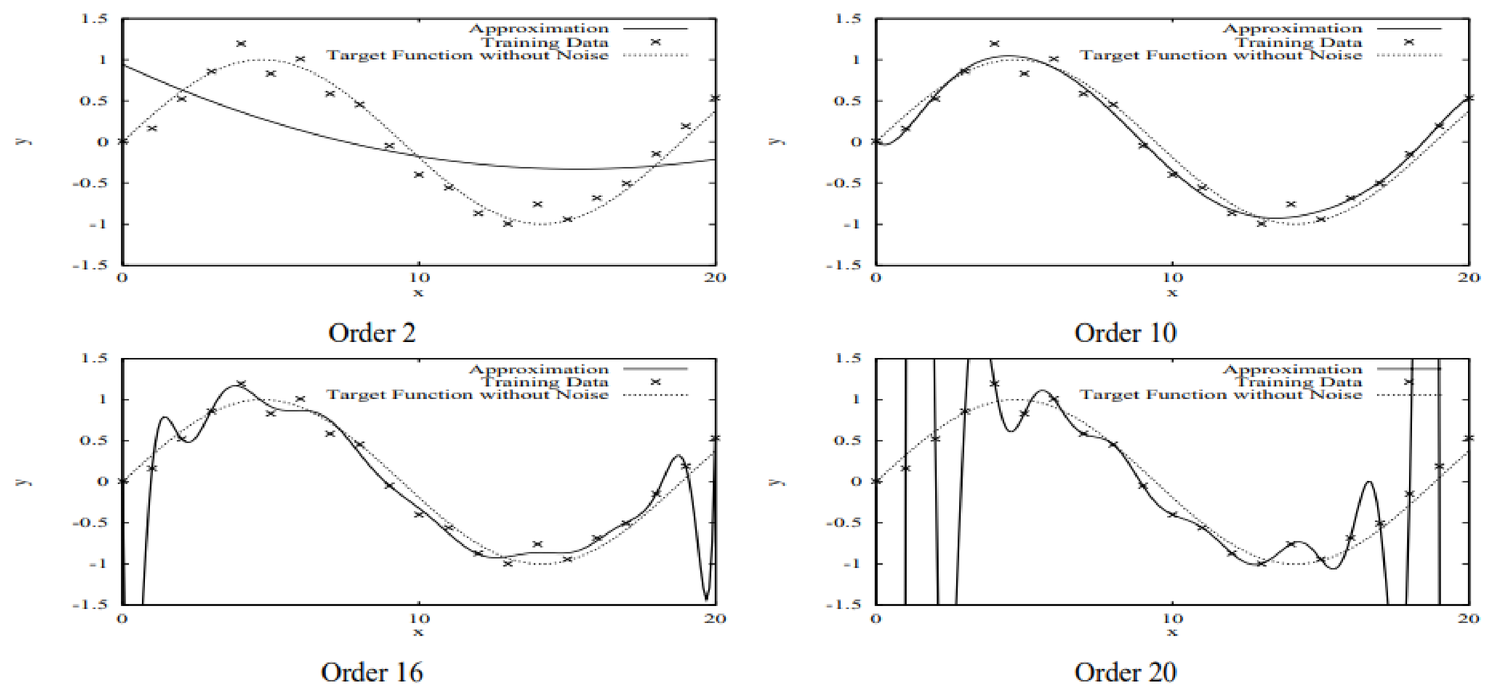
Problem of Overfitting

- Function y = sin(x) is shown by dotted lines
- 21 data points generated by adding random noise
- The data points were fit using polynomials or order 2, 10, 16, and 20

$$\hat{Y} = c_o + c_1\, x + c_2\, x^2 + . . . + c_n\, X_3$$

- Underfit models do not show the right trends
- In Overfit models, the model learns more about data than the trends. In other words, the prediction between the data points may be very erroneous.

Steve Lawrence and C. Lee Giles. Overfitting and Neural Networks: Conjugate Gradient and Backpropagation, International Joint Conference on Neural Networks, Como, Italy, July 24–27, IEEE Computer Society, Los Alamitos, CA, pp. 114–119, 2000

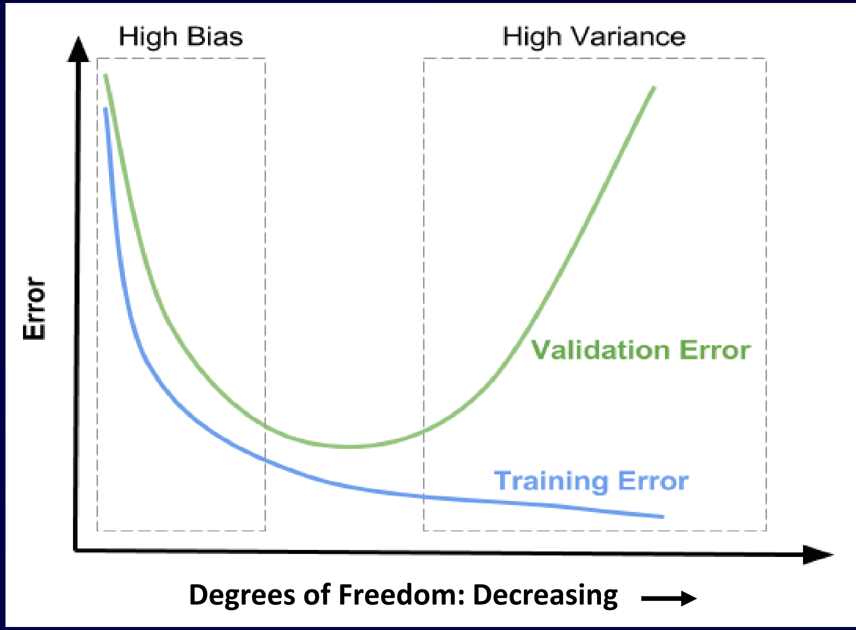


Order	2	10	16	20
# of Parameters	3	11	17	21
Degrees of Freedom	18	10	4	0
Fit	Under	Right	Slightly Overfit	Overfit

Model Accuracy: Validation Datasets

- Hold-Out Validation
  - Dataset is split into Training and Validation datasets
  - Model is trained using Training Dataset and Error is calculated
  - Model is then run using Validation Dataset. Validation Error should not be significantly higher than Training Error

- K-Fold Cross Validation
  - The original dataset is split into K # of portions
  - The training and validation process is repeated k times
  - Each portion takes turn as Validation Dataset while the remaining data portions are used as Training Dataset
  - The model is finally trained with the original data as Training Dataset.



https://dziganto.github.io/cross-validation/data%20science/machine%20learning/model%20tuning/python/Model-Tuning-with-Validation-and-Cross-Validation/

- High Bias: error due to model's inability to learn from data
- High Variance: high validation error due to overfitting
- Model complexity increases as number of neurons and layers increase

Model Accuracy: Statistical Analysis

1. Degrees of freedom

$$\gamma = N_d - N_p$$

2. Sum of Squares of Total Error

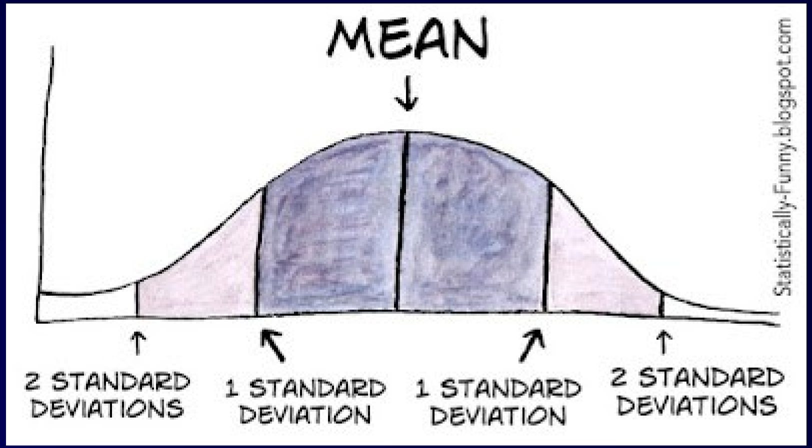
$$SST = \sum_1^{N_d} (y_i - \overline{y})^2$$

3. Sum of Squares of Residuals (Estimation Error)

$$SSR = \sum_1^{N_d} (y_i - \hat{y})^2$$

4. Standard Deviation of Estimates

$$\hat{\sigma} = \sqrt{\frac{SSR}{N_d - N_p}}$$



https://statistically-funny.blogspot.com/2013/04/dont-worry-its-just-standard-deviation.html

5. Coefficient of Determination

$$R^2 = 1 - SSR/SST$$

6. Prediction Interval (95% Confidence)

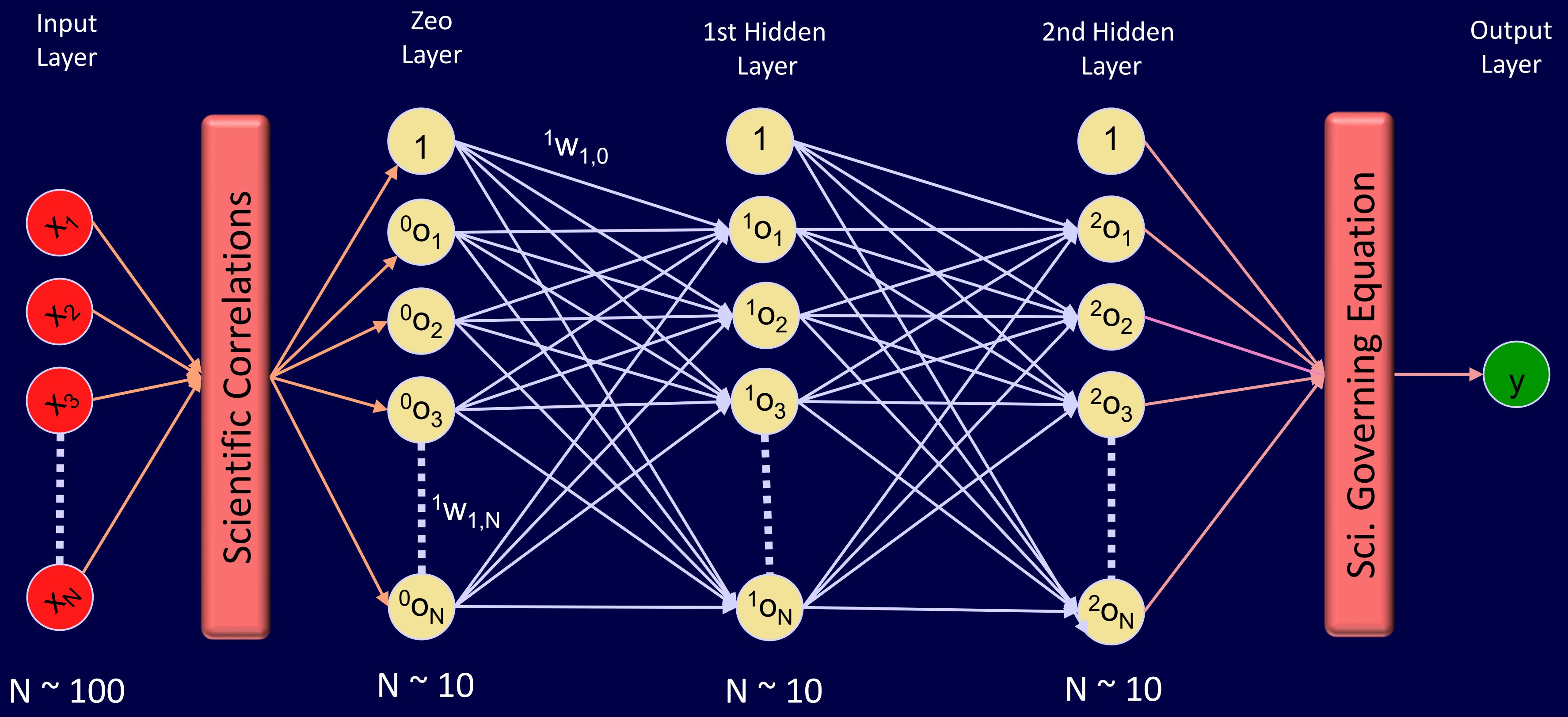
$$y \cong \hat{y} \pm 1.96\,\hat{\sigma}$$

* Regression statistics cannot take into account the effect of number of iterations. Also, Eq. 6 should be applied to Neural Network with caution

Intugent

New Trends in AI for Material Sci. Applications
Scientific Artificial Intelligence (sAI)

- Each solid grey line represents a parameter that needs to be optimized during training
- sAI require smaller datasets for training while giving more accurate trends
- It can be used for new materials before collecting significant data



Different Types of Predictive Models

Artificial Intelligence (AI) Models

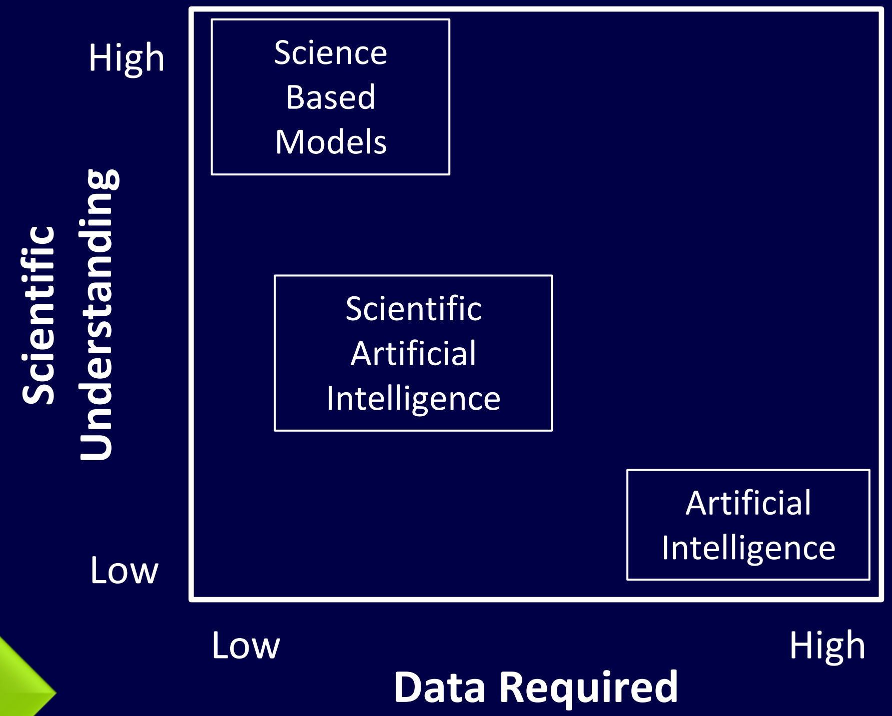
Recipe → Artificial Intelligence → Properties

Science Based Models

Recipe → Formulation Descriptors → Governing Equation → Properties

<u>INTUGENT APPROACH</u>: scientific Artificial Intelligence (sAI) Models

Recipe → Formulation Descriptors → Artificial Intelligence → Governing Equation → Properties



Scientific Artificial Intelligence models combine science and Artificial Intelligence. They require relatively smaller datasets and predict more accurate trends

Part 3

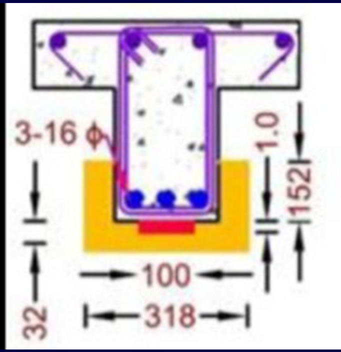
Case Studies

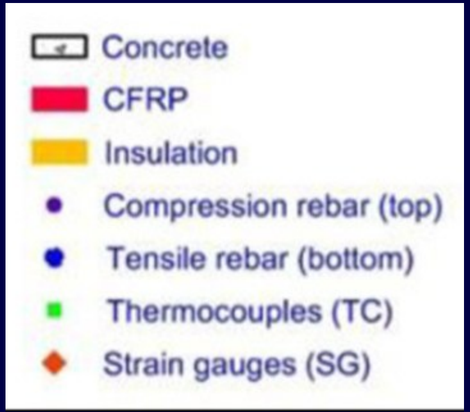
https://cloud.google.com/products/ai/ml-comic-1

CS1: Fire Resistance of FRP-Strengthened Concrete Beams

(Bhatt et. al., https://doi.org/10.1016/j.dib.2024.110031)

ID	Length	Area Conc.	Conc. Cover	Area Steel	Area FRP	Thick Ins.	Height Ins.	Mod Conc.	Yield. Str.	Mod. Steel	Ten. Str. Steel	Mod. FRP	T_g Poly.	Th. Cond.	Heat Cap. Ins.	Load	Load Ratio	Deflec-tion
	(m)	(mm^2)	(mm)	(mm^2)	(mm^2)	(mm)	(mm)	(MPa)	(MPa)	(MPa)	(MPa)	(MPa)	°C	(W/mK)	(J/°Cm^3)	kN	(%)	(mm)
B1	3	60000	25	402.1	0	0	0	47.6	591	205000	0	0	0	0	0	61.2	44.8	-55.81
B2	3	60000	25	402.1	0	0	0	45.5	591	205000	0	0	0	0	0	61.2	44.8	-48.67
B3	3	60000	25	402.1	120	25	0	44.4	591	205000	2800	165000	52	0.175	730800	81.2	38.4	-57.12
B4	3	60000	25	402.1	120	40	80	47.4	591	205000	2800	165000	52	0.175	730800	81.2	38.4	-15.24
B5	3	60000	25	402.1	120	25	80	45.1	591	205000	2800	165000	52	0.175	730800	81.2	38.4	-26.64
B6	3	60000	25	402.1	120	0	0	46	591	205000	2800	165000	52	0.175	730800	81.2	38.4	-31.7
B45	3.66	125730	38	603.2	173.4	0	0	42	440	210000	1034	73770	82	0	510000	98	51	-84
B46	3.66	125730	38	603.2	173.4	25	75	42	440	210000	1034	73770	82	0.156	510000	98	51	-65
B47	3.66	125730	38	603.2	173.4	19	112	42	440	210000	1034	73770	82	0.156	510000	116	61	-108
B48	3.66	125730	38	603.2	102	32	152	46	460	210000	1172	96500	82	0.156	510000	97	51	-16
B49	3.66	125730	38	898	102	19	152	46	450	210000	1172	96500	82	0.156	510000	128	54	-30

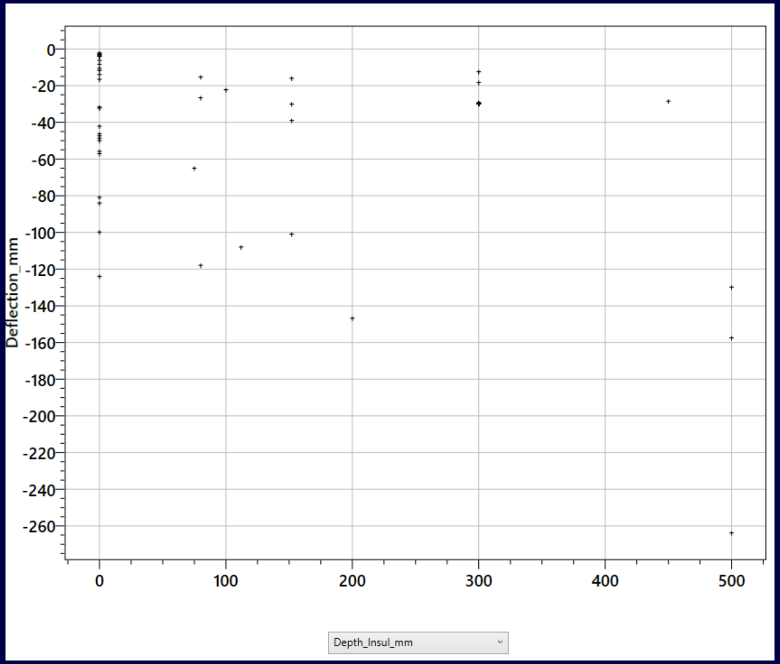




- 17 input variables, 49 data points and 1 replicate
- Must reduce the # of variables

CS1: Fire Res. FRP-Conc. Beams – Deflection Time

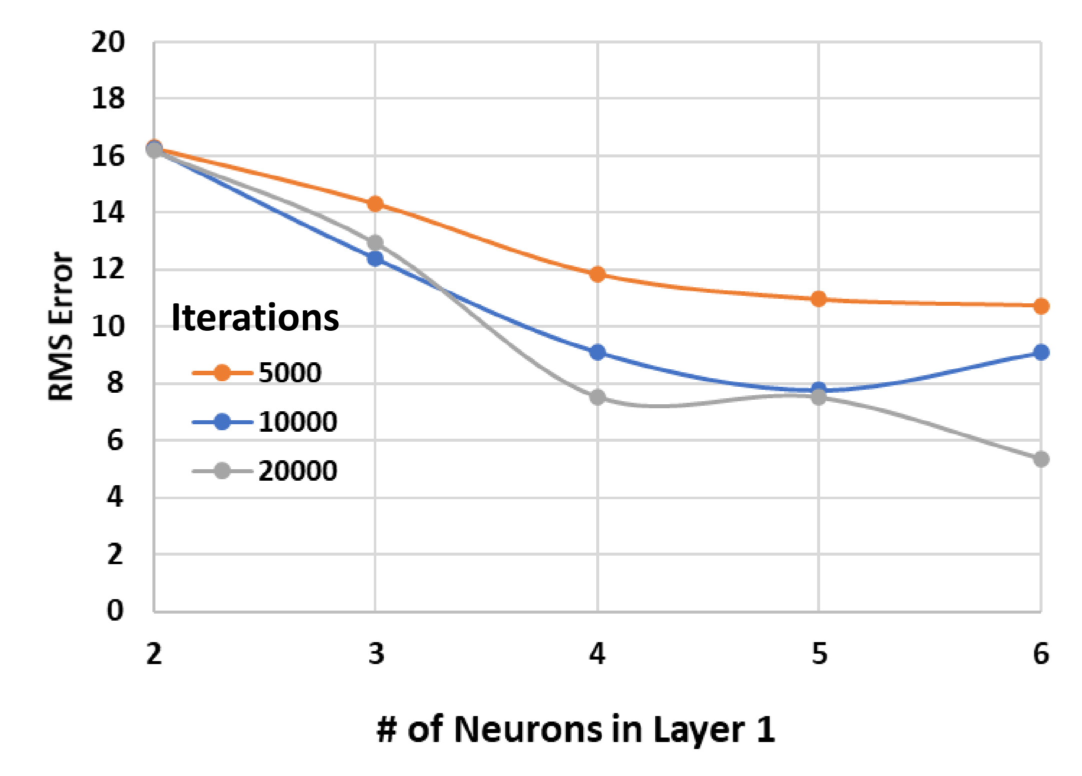
Variable	Average	St. Dev.	Coeff. Corr.
Length_m	2.86	1.23	-0.74
YieldStr_Steel_Mpa	503.2	68.6	0.67
Area_Steel_mm2	319.9	276.8	-0.65
Load_kN	58.92	37.57	-0.60
Area_Conc_mm2	55,170	38,228	-0.59
Depth_Insul_mm	119.7	156.6	-0.41
Cover_Conc_mm	21.08	8.15	-0.25
Thick_Insul_mm	21.71	16.23	0.24
Load_Ratio_%	34.79	20.87	-0.23
TensileStr_FRP_MPA	2,125	1,167	-0.16
ThCond_Insul_W/m-K	0.12	0.15	0.13
Mod_Steel_Mpa	200,304	29,352	-0.12
ThermCap_Insul_J/C-m3	441,291	321,903	0.11
Tg_FRP_C	56.50	26.18	-0.06
Mod_FRP_MPA	160,978	134,564	0.06
Area_FRP_mm2	67.83	71.95	0.05
Mod_Conc_Mpa	36.74	8.02	0.03



Variables Used for Modeling

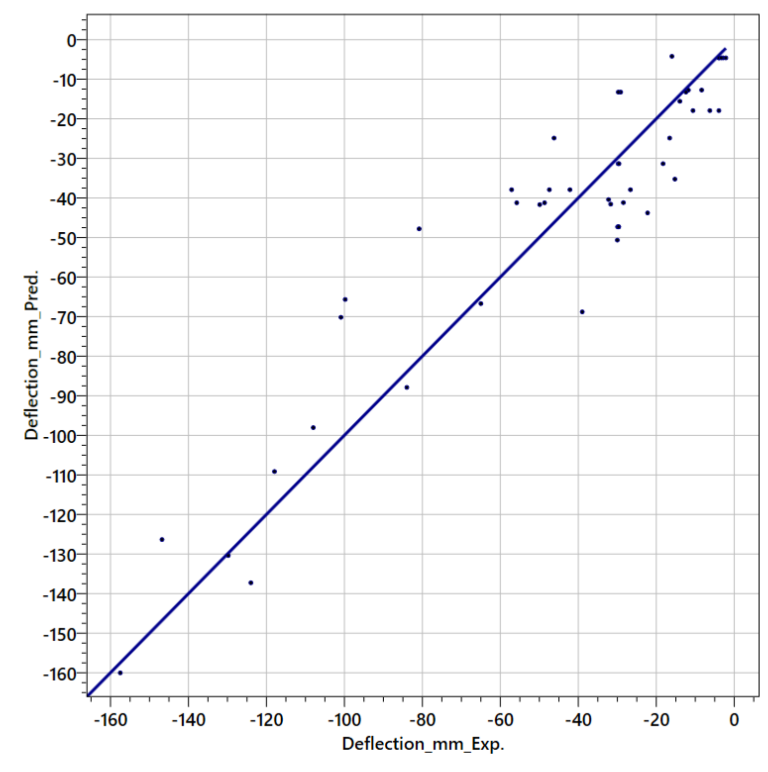
1. Length_m * Area_Conc_mm2 as 'Volume_Conc'
2. [Load_kN]* [Load_Ratio_%] as 'Load*Ratio'
3. [Thick_Insul_mm]
4. [Cover_Conc_mm]
5. [YieldStr_Steel_Mpa]

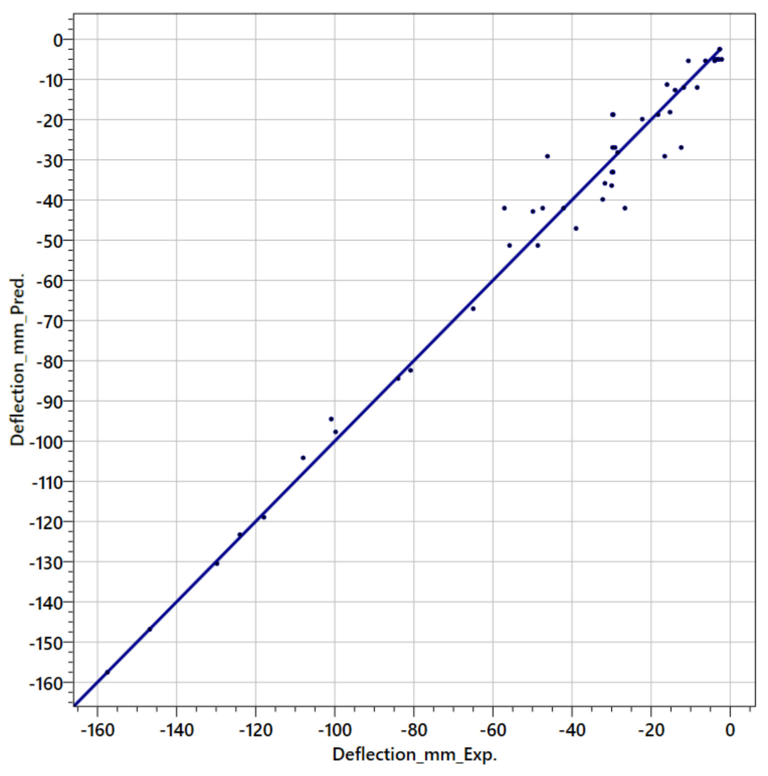
CS1: Fire Res. FRP-Conc. Beams – Model Convergence



- Increase in # of Neurons
  - Increases # of parameters to be optimized
  - Decreases degrees of freedom
  - Reduces root mean square error
  - Initially decreases, but then increases standard deviation
  - Initially improves, but then reduces the quality of predictions
- Increase in # of iterations
  - Reduces root mean square error
  - Reduces standard deviation
  - Initially improves, but then may reduce the quality of predictions as the model starts remembering the points and not the trends

CS1: Fire Res. FRP-Conc. Beams – Neural Network Model





# of Hid. Layers = 1
# of neurons = 2
Deg. of Freedom = 29

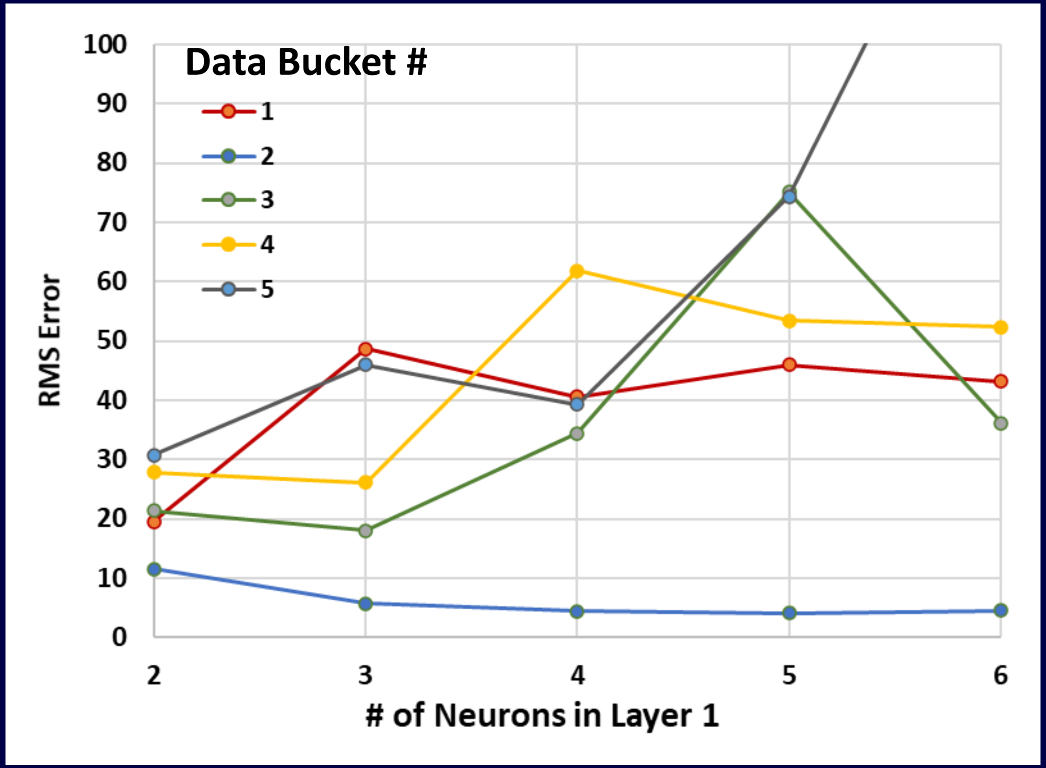
Total # of Iterations	5000
RMS Error	1.5661E+001
Coefficient of Determination (%)	90.48
Standard Deviation of Estimates	20.564

# of Hid. Layers = 1
# of neurons = 6
Deg. of Freedom = 1

Total # of Iterations	20000
RMS Error	6.1089E+000
Coefficient of Determination (%)	98.55
Standard Deviation of Estimates	43.197

CS1: Fire Res. FRP-Conc. Beams – Model Cross Validation

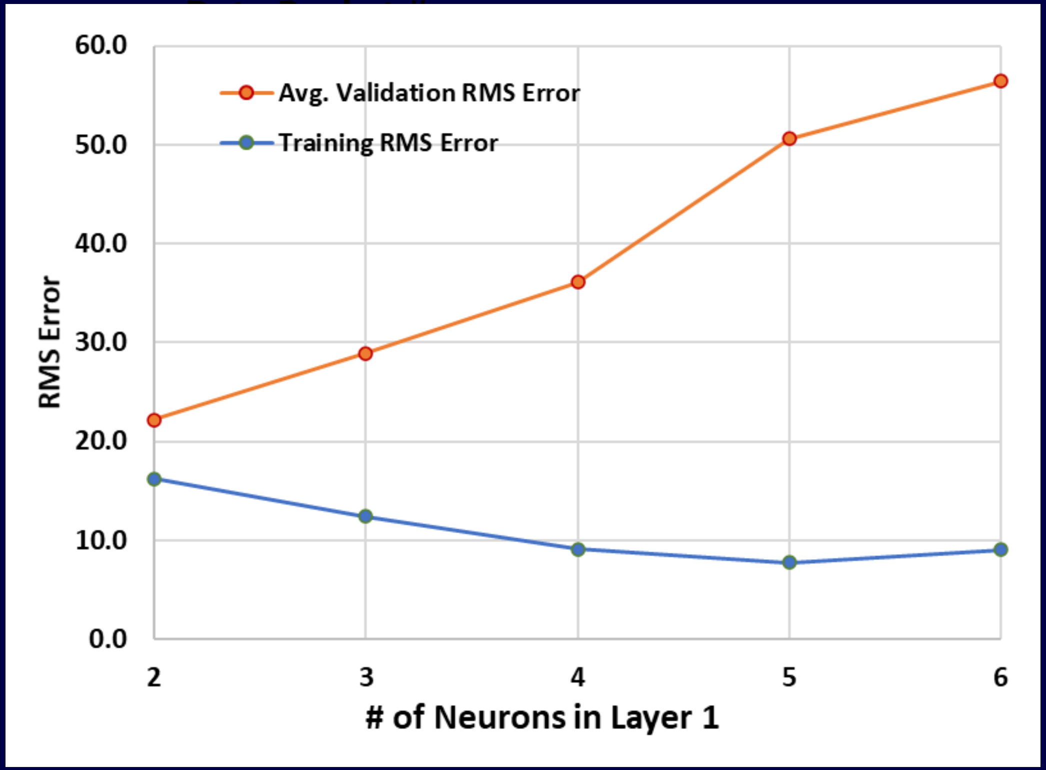
Validation RMS Error with 1000 Iteration.



- Data was divided into 5 buckets
- Each time, 4 out of 5 buckets were used to train the model and the 5th was used to validate the model
- The graph shows the RMS Error when each bucket was used to validate the model
- In general, validation error increased as number of neurons increased (degrees of freedom decreased

CS1: Fire Res. FRP-Conc. Beams – Model Cross Validation

Training vs. Avg. Validation Error (1000 Iteration)



- Use the least # of neurons that can give acceptable error
- In general, there should be more than 3 data points for every adjustable parameter
- Stop training the model as convergence slows down
- Use average Validation Error as guide for model acceptance

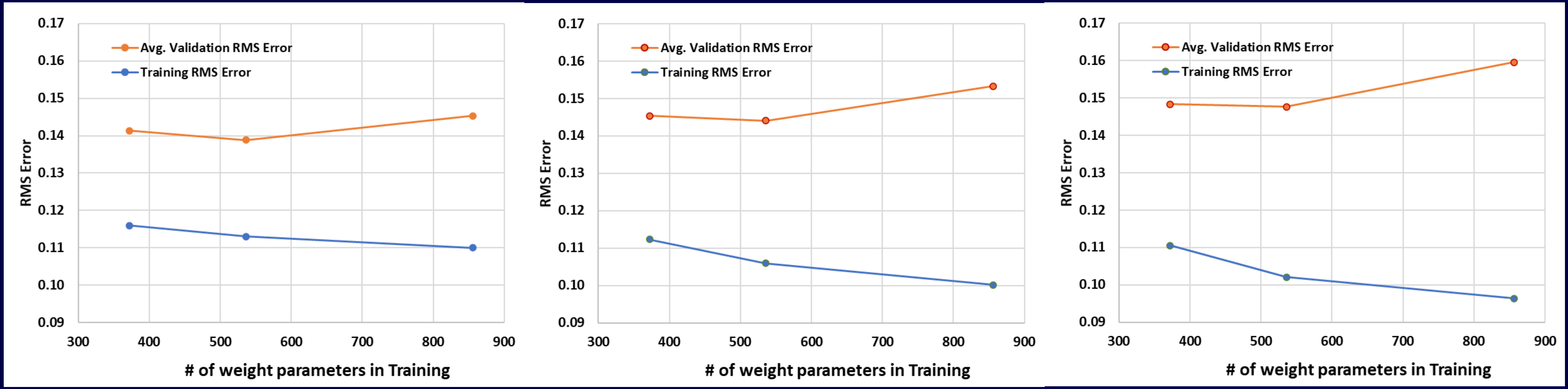
CS2: Real Life Mfg. and Quality Data

- Objective: predict quality control variable (Y) using the process variables (X1, X2, …, X23)
- Data obtained from a real-life manufacturing facility
- Data is scaled to the 0-1 range and process variables names omitted for confidentiality
- 23 input variables with Coeff. of Correlation > 0.05

Variable	Average	St. Dev.	Coeff. Corr.
X1	0.568	0.229	-0.397
X4	0.432	0.236	-0.316
X21	0.714	0.221	0.305
X7	0.342	0.146	-0.303
X2	0.525	0.265	-0.302
X23	0.322	0.182	-0.297
X3	0.469	0.263	-0.289
X5	0.421	0.154	-0.283
X6	0.387	0.150	-0.252
X16	0.444	0.192	0.225
X19	0.551	0.191	0.211
X15	0.503	0.178	0.208
X18	0.435	0.152	0.204
X14	0.491	0.182	0.201
X17	0.381	0.139	0.196
X22	0.411	0.148	0.192
X20	0.418	0.187	0.070
X11	0.399	0.219	-0.058
X13	0.400	0.219	-0.058
X12	0.400	0.219	-0.057
X8	0.385	0.197	-0.055
X10	0.385	0.197	-0.055
X9	0.389	0.195	-0.053

CS2: Mfg. & Qual. Data – Training vs Validation Error

Iterations 5,000 10,000 15,000

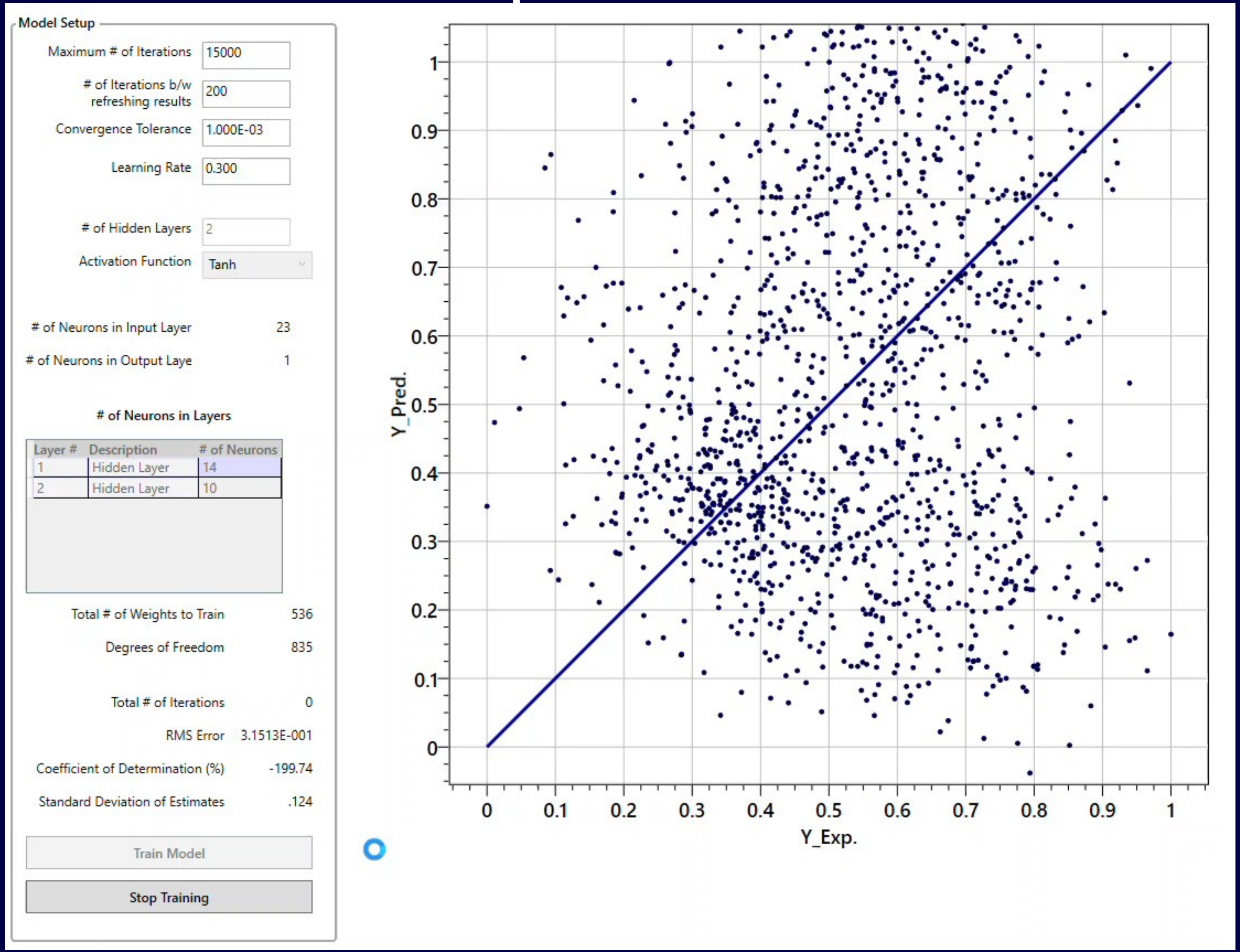


- Data was divided into 5 buckets
- Each time, 4 out of 5 buckets were used to train the model and the 5th was used to validate the model
- Two hidden layers with (10,8), (14,10) & (20, 15) neurons were tried
- The gap b/w training and validation errors slightly increased with # of neurons & # of iterations

CS2: Mfg. & Qual. Data – Model Training in Action

- 23 input variables
- 2 Hidden Layers with 14 & 10 neurons
- 1713 data points
- 536 weight parameter to be trained
- 1177 degrees of freedom
- After 1500 iterations
  - 0.0957 RMS error
  - 72.30 Coeff. of Determination
  - 0.123 Std. Dev. of Estimates

Real Time Screen Capture



CS3: Predicting Young's Modulus of Elastomeric Polyurethanes from the Material Recipe

- Wide range of applications in Coatings, Adhesives, Sealants, and Elastomers
- Experimental data is not available
- Data was synthesized using the scientific math model developed by Ginzburg et. al.*
- Each formulation contained up to five different Polyols, one Chain Extender, and one Isocyanate
- Three thousand different formulations were synthesized using 51 different polyols, 10 chain extenders, and 11 isocyanates with iso index of 100

* Ginzburg et. al., "Theoretical Modeling of the Relationship between Young's Modulus and Formulation Variables for Segmented Polyurethanes," Journal of Polymer Science: Part B: Polymer Physics, Vol. 45, 2123–2135, (2007).

CS-3: Mod. of Flex. PU – Input Data

Table 1A: Polyols

Name	OH#	Func.
VORANOL™ 1010 L	110.0	2
VORANOL 2000 L	56.5	2
VORANOL 2110-B	110.0	2
VORANOL 2110-TB	110.0	2
VORANOL 2120	56.1	2
VORANOL 2120 L	56.0	2
VORANOL 2120 P	56.0	2
VORANOL 2140	27.9	2
VORANOL 220-028	27.9	2
VORANOL 220-056	56.0	2
VORANOL 220-056 N	56.0	2
VORANOL 220-110	110.0	2
VORANOL 220-110 N	110.0	2
VORANOL 220-260	260.0	2
VORANOL 222-029	28.7	2
VORANOL 222-056	56.0	2
VORANOL 223-060 LM	61.0	2
VORANOL 230-112	112.0	3
VORANOL 4240	28.7	2
VORANOL B 2000	56.0	2
VORANOL EP 1900	27.5	2
VORANOL P 400	260.0	2
VORANOL P 4000	27.9	2
VORANOL WD 2104	270.0	2
VORANOL WD 2130	37.5	2
VORAPEL D3201	56.1	2

Table 1A: Contd.

Name	OH#	Func.
VORANOL 1000 LM	112.0	2
VORANOL 2000 LM	56.0	2
VORANOL 222-028 LM	56.0	2
VORANOL 3000 M	37.0	2
VORANOL 3003 LM	56.0	2
VORANOL 4000 LM	28.0	2
VORANOL 8000 LM	14.0	2
POLYOL 355 UCB	158.0	3
VORANOL 2070	236.2	3
VORANOL 2100	56.0	3
VORANOL 230-042N	43.0	3
VORANOL 230-056	56.0	3
VORANOL 230-238	236.2	3
VORANOL 230-660	660.0	3
VORANOL 231-027N	26.0	3
VORANOL 232-028	28.0	3
VORANOL 232-034	33.0	3
VORANOL 232-034N	34.0	3
VORANOL 232-036N	36.0	3
VORANOL 2471	33.0	3
VORANOL 270	237.0	3
VORANOL 271C	33.0	3
VORANOL 410	0.0	3
VORANOL 450N	383.0	3
VORANOL 5055 HH	29.0	3

Table 1B: Chain Extenders

Name	OH#	Func.
1,4-BUTANEDIOL	1247	2
2-ETHYL 1,3 HEXANEDIOL	1247	2
DiethanoLAMINE	1069	3
Diethylene Glycol	1058	2
Ethylene Glycol	1810	2
ETHACURE 100 (DETDA)	1069	2
GLYCERINE - NATURAL	1829	3
PROPYLENE GLYCOL	1476	2
TRIETHYLENE GLYCOL	748	2
TRIMETHYLOLPROPANE	1256	3

Table 1C: Isocyanates

Name	%NCO	Func.
Isophorone diisocyanate	37.7	2.0
ISONATE™ M 340 modified pu	26.3	2.1
ISONATE OP 20 Pure MDI	33.5	2.0
ISONATE OP 30 Pure MDI	33.5	2.0
ISONATE OP 50 Pure MDI	33.5	2.0
PAPI™ 901	31.8	2.3
PAPI 95	31.5	2.3
PAPI 94 Polymeric MDI	32.1	2.3
PAPI 27 Polymeric MDI	31.6	2.7
PAPI 580N Polymeric MDI	30.9	3.0
VORANATE™ T80	48.2	2.0

* Polyols selected from Customized options for a range of CASE applications, Dow website https://www.dow.com/en-us/product-technology/pt-polyurethanes/pg-polyurethanes-polyols.html#tabs-1ea19b782b-item-c0fd89c605-tab

- If these material are directly used as input, the input layer will have at least 72 neurons
- Dimensionality reduction using Formulation Descriptors can reduce the total number of parameters to be trained

CS-3: Mod. of Flex. PU – Understanding Molecular Structure

- Elastomeric PU find various applications in Adhesives, Coatings, Sealants & Elastomers

- Co-block polymer consists of hard and soft segments

- A typical formulations consist of 1 or more of each of polyols, chain extenders, and Isocyanates as well as additives such as surfactants, pigments, …

- Hard segments phase separate. The morphology primarily depends upon the formulation


1. Spherical*


2. Cylindrical*


3. Gyroid*


4. Lamellar*

* K. Matyjaszewski and M. Muller, Polymer Science: A Comprehensive Reference, pp 129-140, (2012).

- As hard segment concentration increases, they first phase separate to form Spherical, and Cylindrical, Gyroid, and Lamellar shaped domains

CS-3: Mod. of Flex. PU – Formulation Descriptors

1. Hard Segment Percentage
   Key parameter in determining the phase separated structure and hence the modulus

   - Hard Segment wt. = Isocyanate wt.+ Chain Extenders’ wt. + wt. OH group in Polyols
   - Soft Segment wt. = wt. of Polyols – wt. of OH groups in Polyols

2. Solubility Parameters of Hard and Soft Segments
   - Is a measure of cohesive energy
   - Hansen solubility parameter provides a 3D framework
   - Group contribution theory as outlined by Van Krevelen* was used

$$\boldsymbol{\delta} = \sqrt{\boldsymbol{\delta}_d^2 + \boldsymbol{\delta}_p^2 + \boldsymbol{\delta}_h^2}$$

3. Glass Transition Temperatures of Hard and Soft Segments
   - Is a measure of rigidity of molecular segments
   - Group contribution theory as outlined by Van Krevelen* was used

$$T_g = \sum w_i \, T_{g,i}$$

* D. W. Van Krevelen and N. V., Arnhem, “Properties of Polymers, Their Correlation with Chemical Structure, Their Numerical Estimation and Prediction from Additive Group Contributions,” 4th Edition, Elsevier Amsterdam, ISBN 978-0-08-054819-7, (1989)

CS3: Mod. of Flex. PU – Formulation Descriptors

4. Average OH # of Polyols - OH # = 56,100/Eq. Wt.
    - Is a measure of Soft Segment length
    - Calculated as weight averaged value

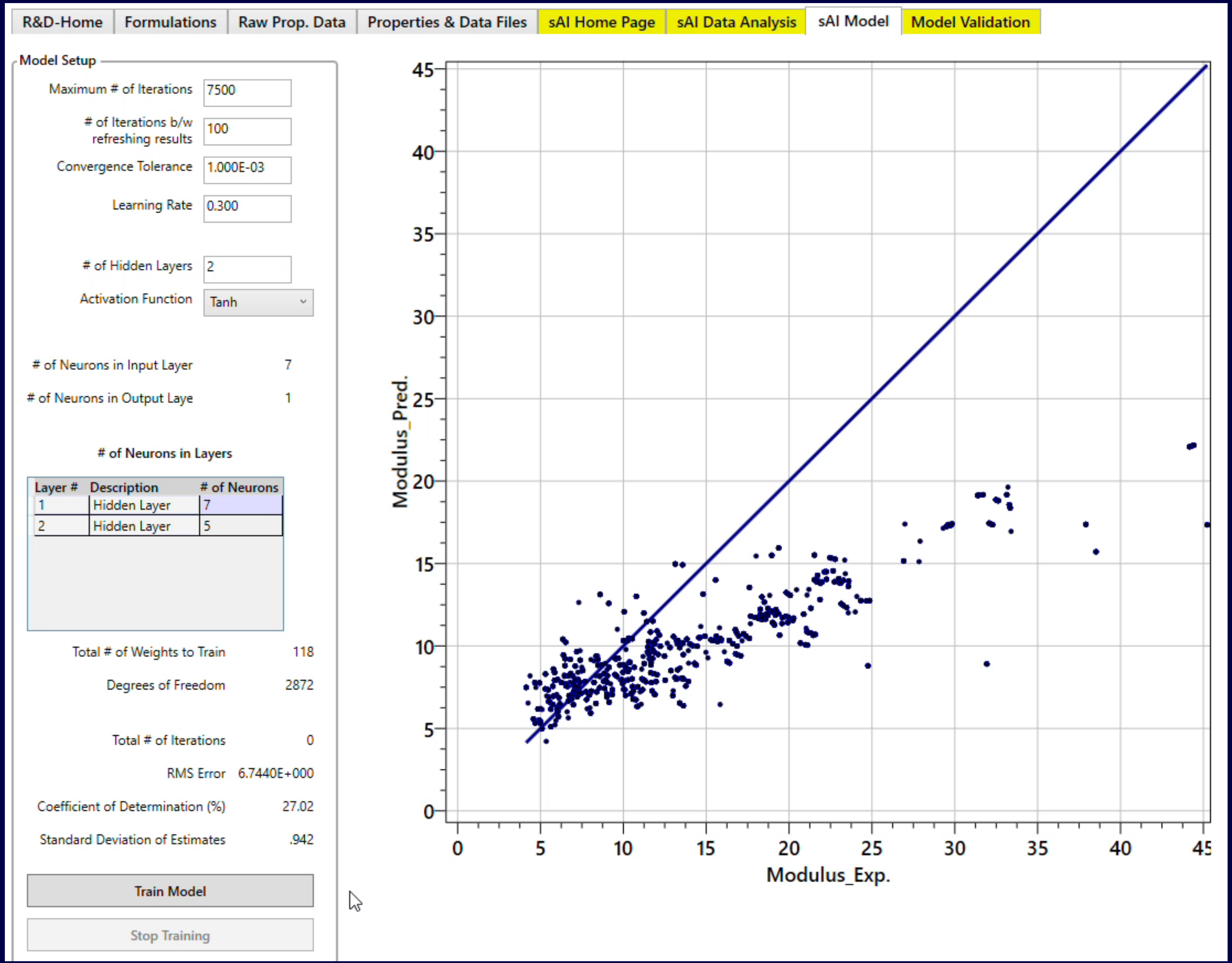
$$OH = \sum w_i \, OH_i$$

5. Average Functionality of Polyols
    - Is a measure of mobility of Soft Segments
    - Calculated as number of equivalents averaged value

$$f = \frac{\sum \frac{w_i \, f_i}{M_{w,i}} f_i}{\sum \frac{w_i \, f_i}{M_{w,i}}}$$

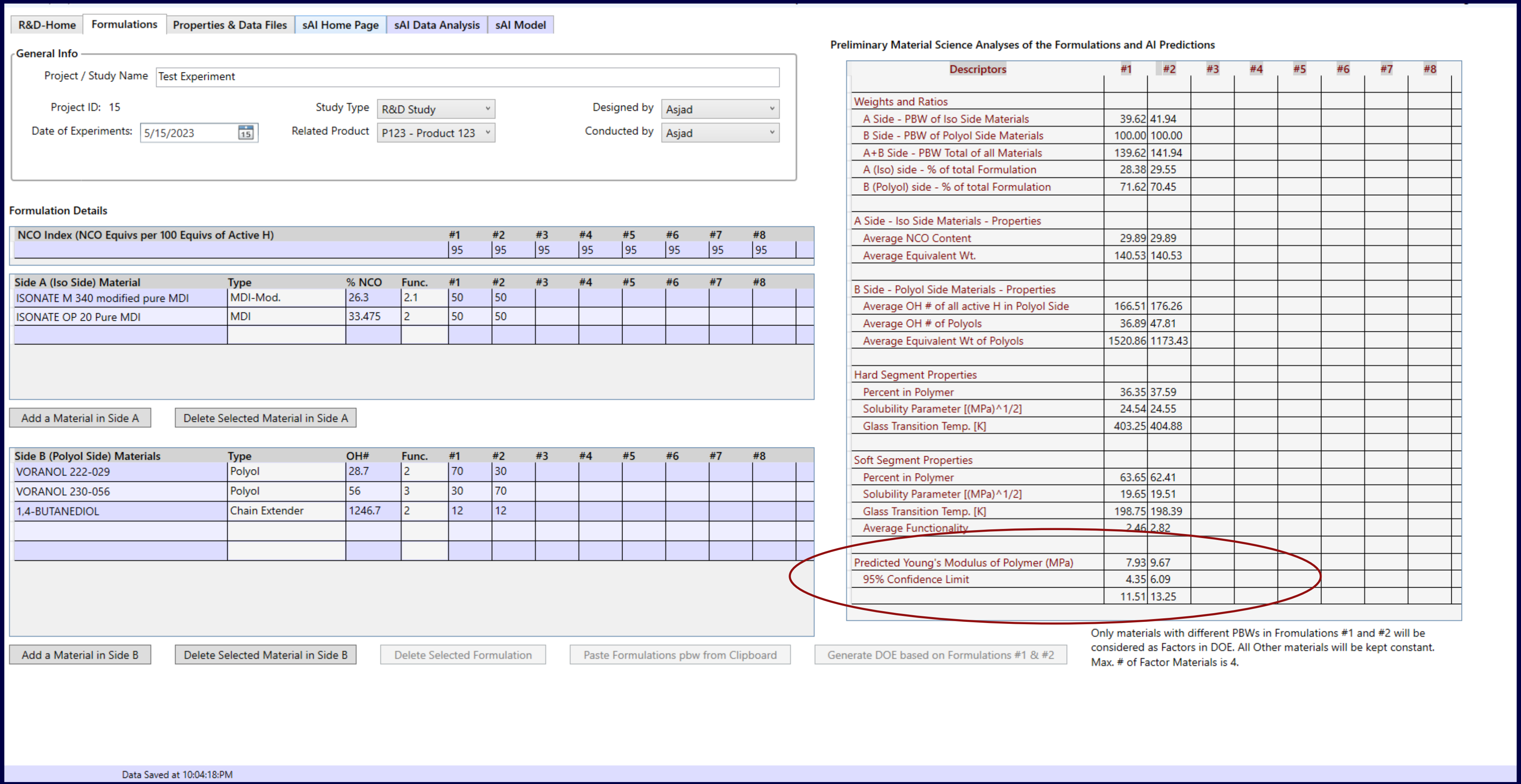
CS3: Mod. of Flex. PU – Model Training in Action

- 7 input variables
- 2 Hidden Layers with 7 & 5 neurons
- 2990 data points
- 118 weight parameter to be trained
- 2872 degrees of freedom
- After 6233 iterations.
  - 0.638 RMS error
  - 99.35 Coeff. of Determination
  - 0.651 Std. Dev. of Estimates



CS4: Digital Transformation-Experiment Setup

Intugent ePI calculates key material science parameters and predicts Modulus using AI model as engineers design new formulations



R&D-Home | Formulations | Properties & Data Files | sAI Home Page | sAI Data Analysis | sAI Model

General Info

Project / Study Name: Test Experiment

Project ID: 15

Date of Experiments: 5/15/2023

Study Type: R&D Study

Related Product: P123 - Product 123

Designed by: Asjad

Conducted by: Asjad

Formulation Details

NCO Index (NCO Equivs per 100 Equivs of Active H)	#1	#2	#3	#4	#5	#6	#7	#8
	95	95	95	95	95	95	95	95

Side A (Iso Side) Material	Type	% NCO	Func.	#1	#2	#3	#4	#5	#6	#7	#8
ISONATE M 340 modified pure MDI	MDI-Mod.	26.3	2.1	50	50						
ISONATE OP 20 Pure MDI	MDI	33.475	2	50	50						

Add a Material in Side A | Delete Selected Material in Side A

Side B (Polyol Side) Materials	Type	OH#	Func.	#1	#2	#3	#4	#5	#6	#7	#8
VORANOL 222-029	Polyol	28.7	2	70	30						
VORANOL 230-056	Polyol	56	3	30	70						
1,4-BUTANEDIOL	Chain Extender	1246.7	2	12	12						

Add a Material in Side B | Delete Selected Material in Side B | Delete Selected Formulation | Paste Formulations pbw from Clipboard | Generate DOE based on Formulations #1 & #2

Preliminary Material Science Analyses of the Formulations and AI Predictions

Descriptors	#1	#2	#3	#4	#5	#6	#7	#8
Weights and Ratios								
A Side - PBW of Iso Side Materials	39.62	41.94						
B Side - PBW of Polyol Side Materials	100.00	100.00						
A+B Side - PBW Total of all Materials	139.62	141.94						
A (Iso) side - % of total Formulation	28.38	29.55						
B (Polyol) side - % of total Formulation	71.62	70.45						
A Side - Iso Side Materials - Properties								
Average NCO Content	29.89	29.89						
Average Equivalent Wt.	140.53	140.53						
B Side - Polyol Side Materials - Properties								
Average OH # of all active H in Polyol Side	166.51	176.26						
Average OH # of Polyols	36.89	47.81						
Average Equivalent Wt of Polyols	1520.86	1173.43						
Hard Segment Properties								
Percent in Polymer	36.35	37.59						
Solubility Parameter [(MPa)^1/2]	24.54	24.55						
Glass Transition Temp. [K]	403.25	404.88						
Soft Segment Properties								
Percent in Polymer	63.65	62.41						
Solubility Parameter [(MPa)^1/2]	19.65	19.51						
Glass Transition Temp. [K]	198.75	198.39						
Average Functionality	2.46	2.82						
Predicted Young's Modulus of Polymer (MPa)	7.93	9.67						
95% Confidence Limit	4.35	6.09						
	11.51	13.25						

Only materials with different PBWs in Fromulations #1 and #2 will be considered as Factors in DOE. All Other materials will be kept constant. Max. # of Factor Materials is 4.

Data Saved at 10:04:18:PM

CS4: Digital Transformation-Experimental / Predicted Data

Experimental results are collected and compared against predictions

R&D-Home | Formulations | Properties & Data Files | sAI Home Page | sAI Data Analysis | sAI Model

Properties of Elastomeric Polyurethanes

	Enter Measured Values								Predicted Values							
Property	**#1**	**#2**	**#3**	**#4**	**#5**	**#6**	**#7**	**#8**	**#1**	**#2**	**#3**	**#4**	**#5**	**#6**	**#7**	**#8**
Hardness ShA	40	50														
Tensile strength [Mpa]	20	25														
Tensile modulus [Mpa]	9.2	10.5							7.93	9.67						
Elongation [%]	600	550														
Abrasion resistance DIN 53516 [mm3]	50	50														
Compression set 70 H @ 212°F [%]																
Compression set 70 H @ -4°F [%]																
Aging 7 days @ 212°F - Tensile strength [%]																
Aging 7 days @ 212°F - Elongation [%]	500	475														
Aging 7 days @ 212°F - Hardness ShA																

Formulation Specific Notes (255 characters max)

Form. #	**Note**
1	Base Case
2	Test 1
3	
4	
5	
6	
7	
8	

Foamat & Other Data Files (*** Enter or paste the file path in the cell. Double Click on the cell to use File Dialogbox ***)

Data / File Type	**#1**	**#2**	**#3**	**#4**	**#5**	**#6**	**#7**	**#8**
FTIR Spectra	C:\Users\Asjad\Desktop\Predict							
TGA		C:\Users\Asjad\Desktop\Case S						
Foamat Data (.csv)								

Data Saved at 10:04:18:PM

CS4: Digital Transformation-Historical Data Relationships

Experimental data collected in the past is analyzed for relationships

R&D-Home | Formulations | Properties & Data Files | sAI Home Page | sAI Data Analysis | sAI Model

General Info

Data/Model Name: Mfg Real Life Data

Database ID: 32

Group

Predicted Property

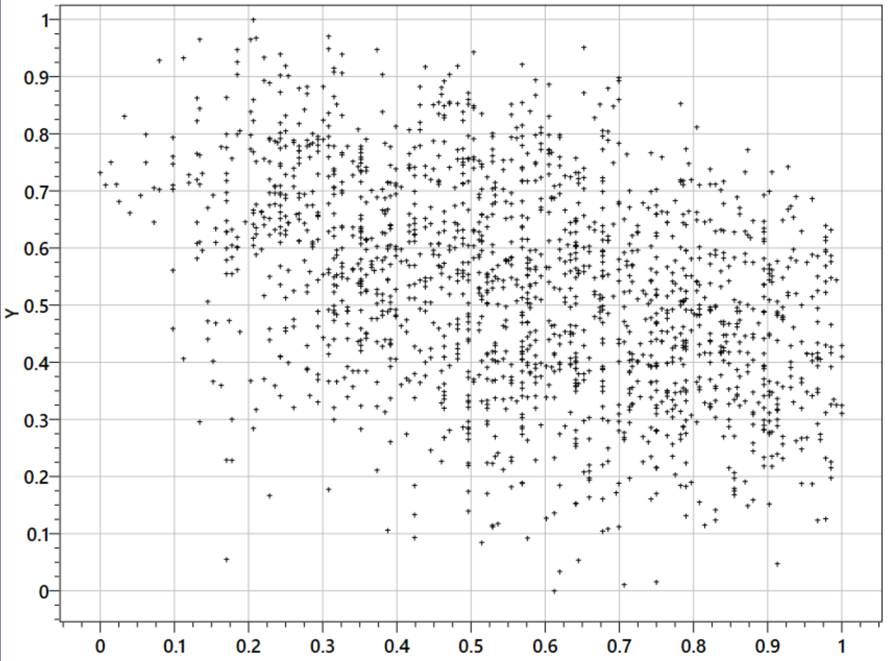
Upload Data

Data Source: SQL Query

Data Source

Browse for Data File

Use SQL Query for: Mfg. Real Life Data



Given Dataset

#	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
0	0.620	0.236	0.063	0.166	0.294	0.302	0.224	0.637	0.640	0.637
1	0.605	0.170	0.040	0.157	0.232	0.249	0.148	0.142	0.148	0.141
2	0.641	0.274	0.122	0.203	0.337	0.362	0.250	0.465	0.476	0.465
3	0.804	0.191	0.055	0.165	0.334	0.361	0.247	0.465	0.471	0.465
4	0.928	0.202	0.139	0.196	0.246	0.297	0.185	0.637	0.640	0.636
5	0.870	0.202	0.128	0.147	0.272	0.264	0.181	0.252	0.257	0.251
6	0.478	0.228	0.111	0.178	0.236	0.295	0.176	0.465	0.470	0.465
7	0.641	0.202	0.125	0.180	0.251	0.298	0.180	0.637	0.640	0.637
8	0.482	0.225	0.122	0.168	0.221	0.270	0.154	0.512	0.516	0.511
9	0.529	0.200	0.128	0.154	0.263	0.290	0.176	0.465	0.469	0.465
10	0.830	0.293	0.136	0.245	0.294	0.373	0.249	0.874	0.875	0.874
11	0.790	0.222	0.124	0.221	0.381	0.396	0.236	0.516	0.520	0.516
12	0.620	0.253	0.162	0.196	0.298	0.268	0.196	0.530	0.533	0.529
13	0.743	0.202	0.122	0.191	0.257	0.276	0.175	0.636	0.640	0.636
14	0.906	0.213	0.128	0.145	0.277	0.288	0.195	0.251	0.257	0.251
15	0.862	0.281	0.159	0.245	0.304	0.362	0.278	0.894	0.895	0.894
16	0.772	0.229	0.121	0.166	0.216	0.315	0.189	0.465	0.469	0.465

Correlation Factors

Variables	Average	StdDev	Correlation
Y	0.5329	0.1820	1.0000
X1	0.5683	0.2294	-0.3967
X4	0.4317	0.2358	-0.3162
X21	0.7141	0.2214	0.3050
X7	0.3424	0.1462	-0.3033
X2	0.5248	0.2652	-0.3023
X23	0.3215	0.1825	-0.2966
X3	0.4690	0.2631	-0.2894
X5	0.4208	0.1537	-0.2830
X6	0.3867	0.1501	-0.2522
X16	0.4442	0.1921	0.2246
X19	0.5505	0.1906	0.2113
X15	0.5033	0.1783	0.2078
X18	0.4354	0.1523	0.2043
X14	0.4907	0.1824	0.2015

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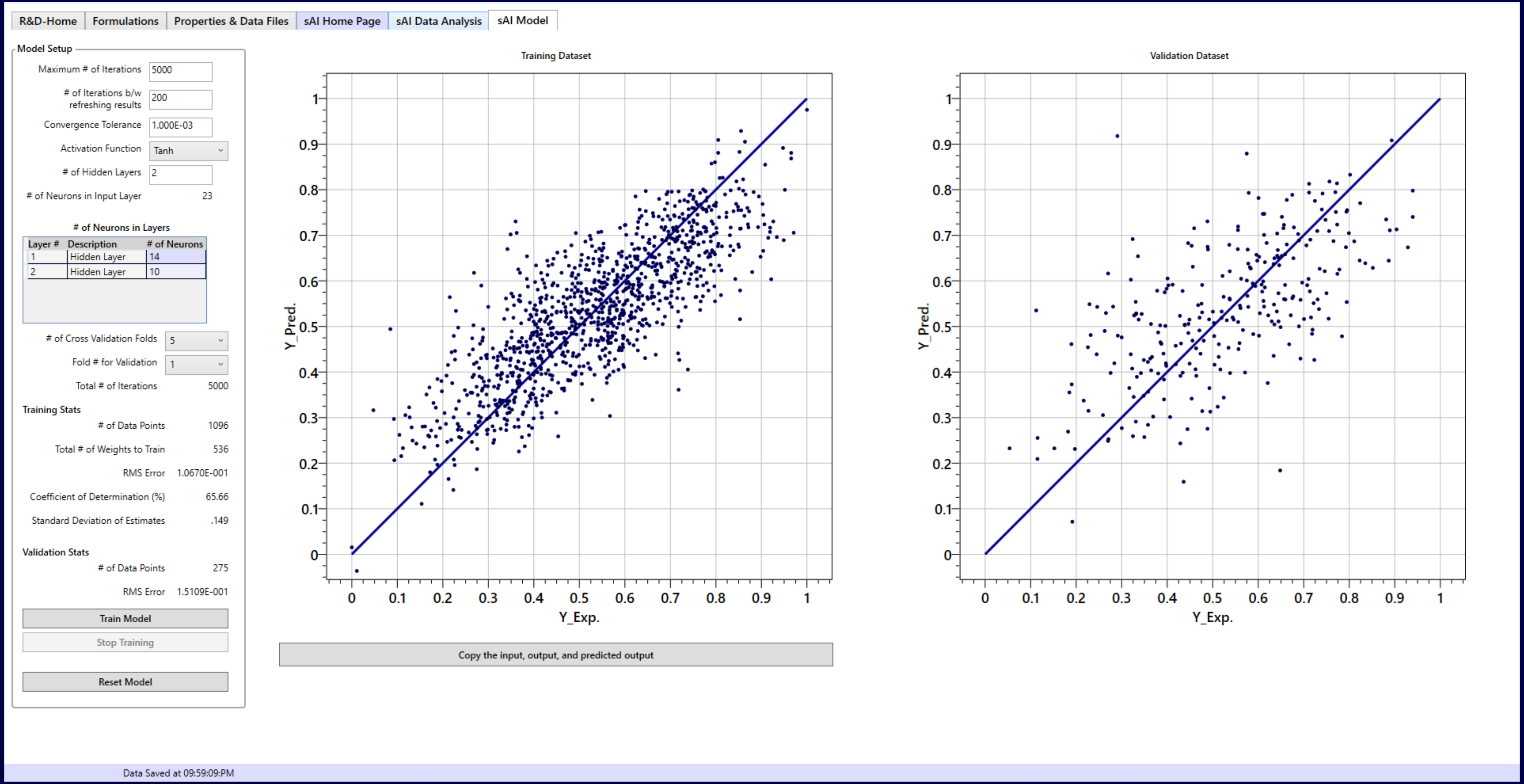
CS4: Digital Transformation-Model Training / Validation

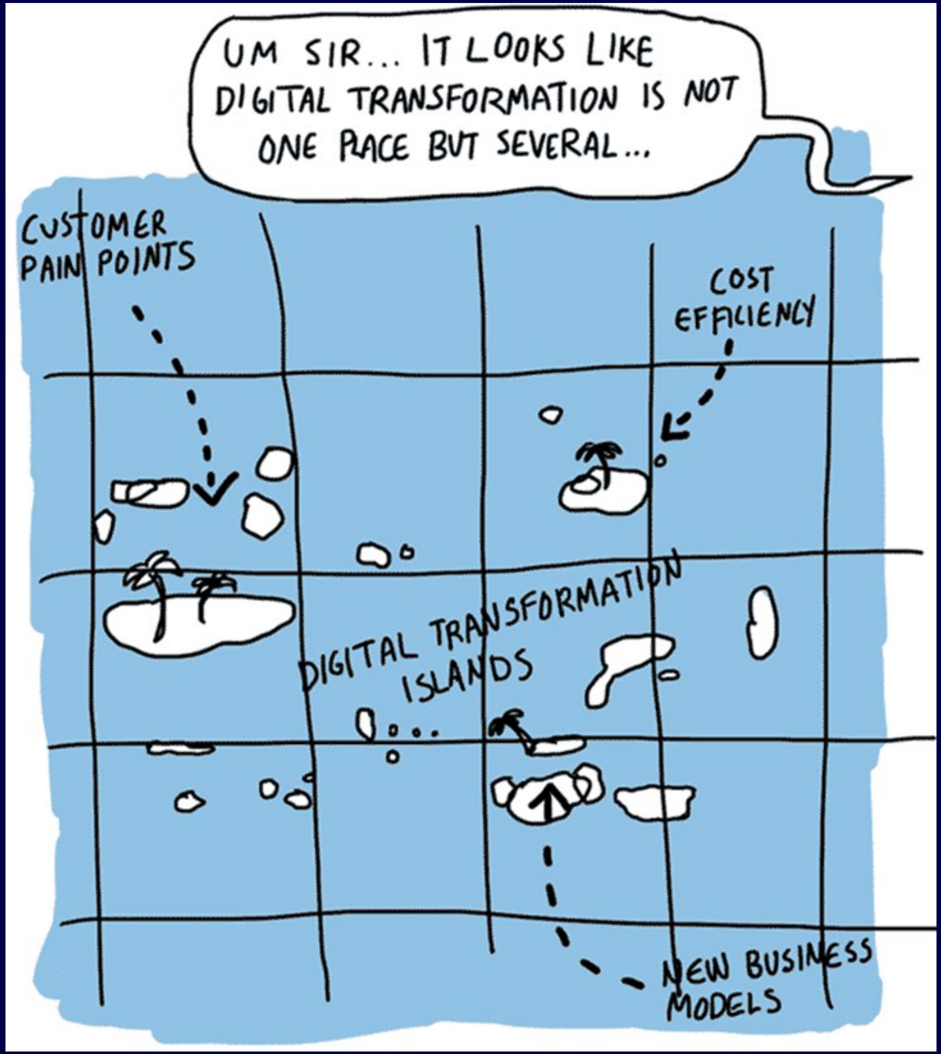
Historical data is used to train AI models and validate them



Part 4

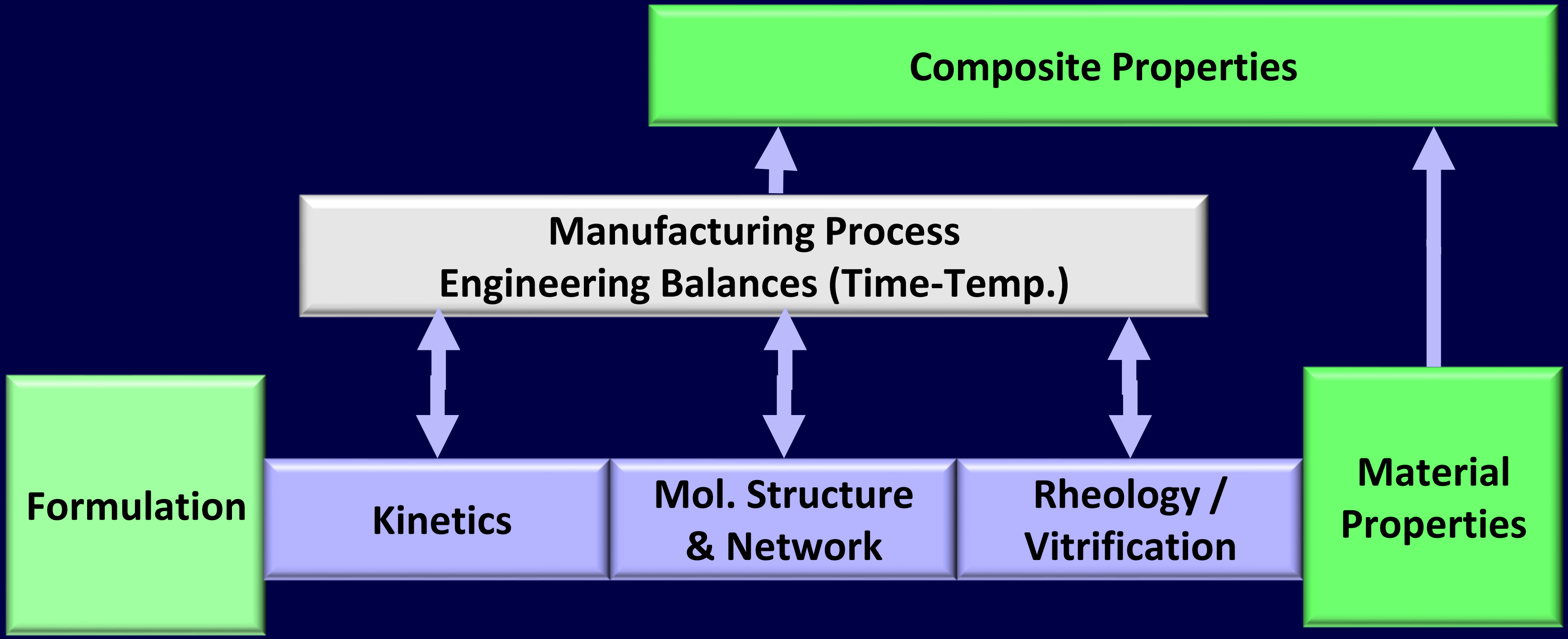
Other Digitalization Techniques

Rheokinetic Models for Scaleup



https://www.businessillustrator.com/what-is-digital-transformation-cartoon-infographic/

Materials Paradigm / Process Domain



Property Prediction Models

- Predict properties after reactions are complete (lab or commercial scale)
- AI & Math Models

Process Simulation Models

- Can we complete processes under commercial application conditions
- Rheokinetic scaleup models

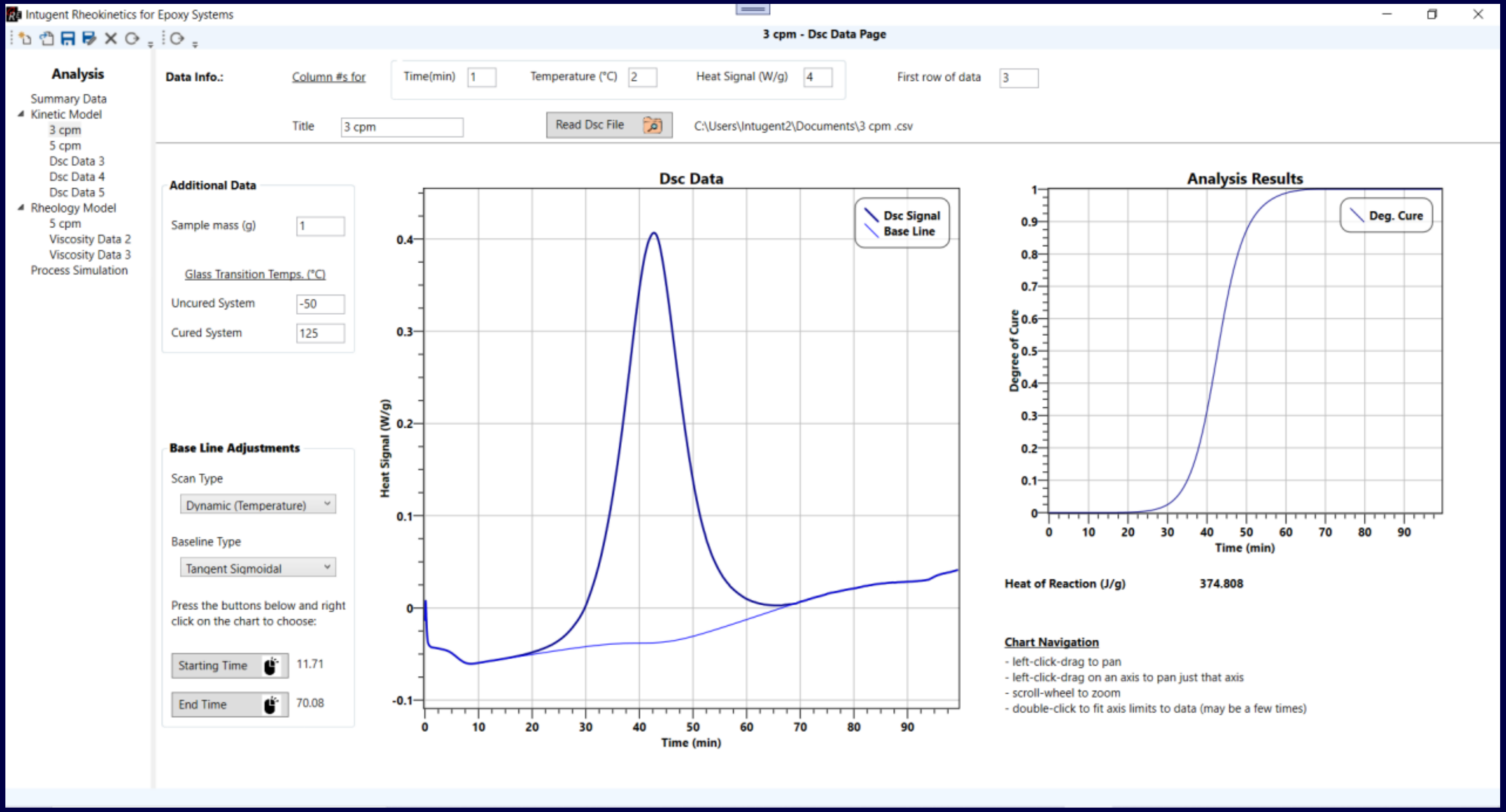
Process Simulation Models

Process Scaleup Models

1. Generate lab scale data in DSC and rheometers and develop Rheokinetic model
   i. At least 2 dynamic DSC scans or 3 isothermal scans
   ii. At least 1 rheology scan

2. Use Rheokinetic model with know temperature profile or with heat transfer equations to simulate the industrial scale process

DSC Scans

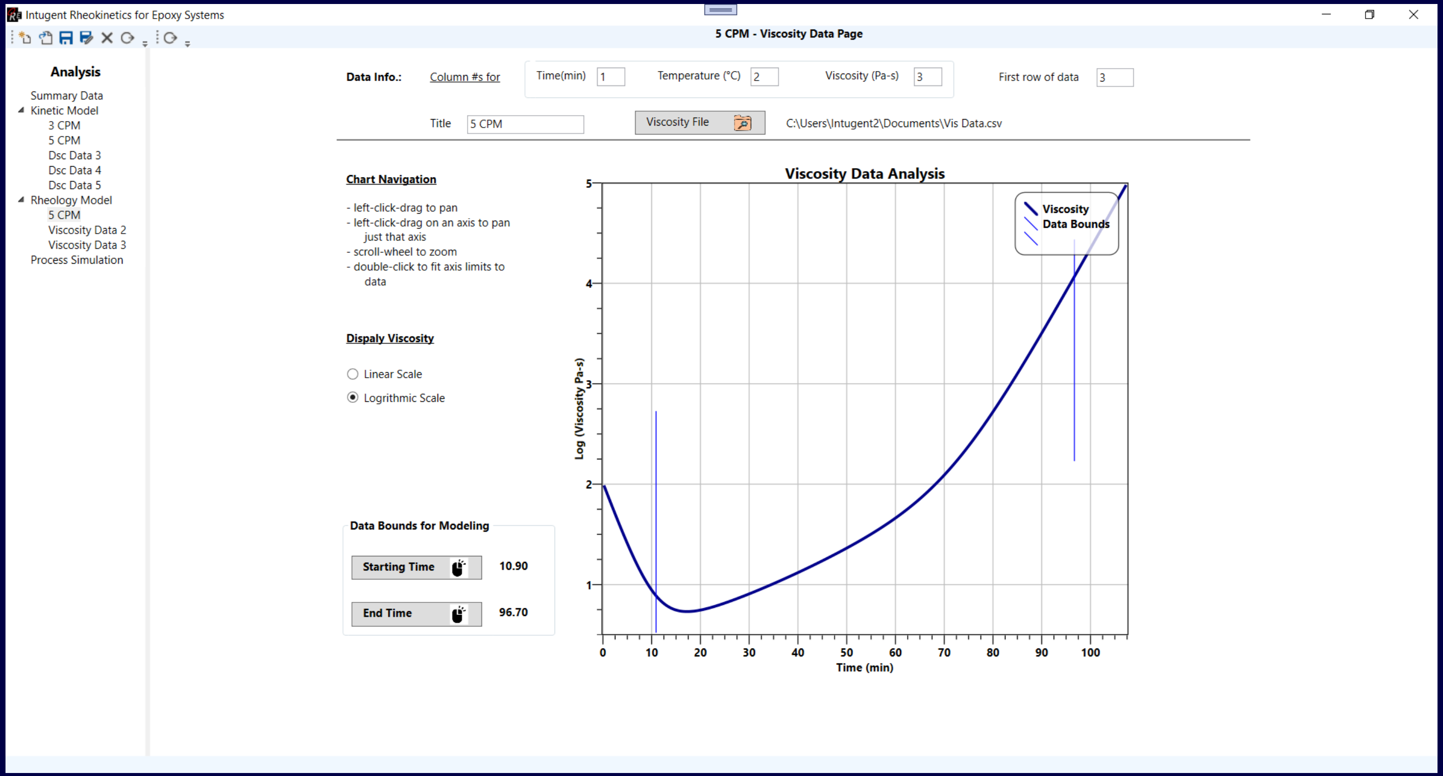


Autocatalytic Kinetic Model

$$\frac{d\alpha}{dt} = (\,k_1 + k_2\,\alpha^{n_2})\,(1-\alpha)^{n_1}$$

- Next generation models take into account the effect of vitrification (glass transition temperature) on reaction kinetics.
- Researchers do not need any background to use this software

Rheology Scans



Castro & Macosko Model

$$\eta = \eta_0 \, exp\left(\frac{E_\eta}{\Re T}\right)\left(\frac{\alpha_g}{\alpha_g - \alpha}\right)^{a+b\alpha}$$

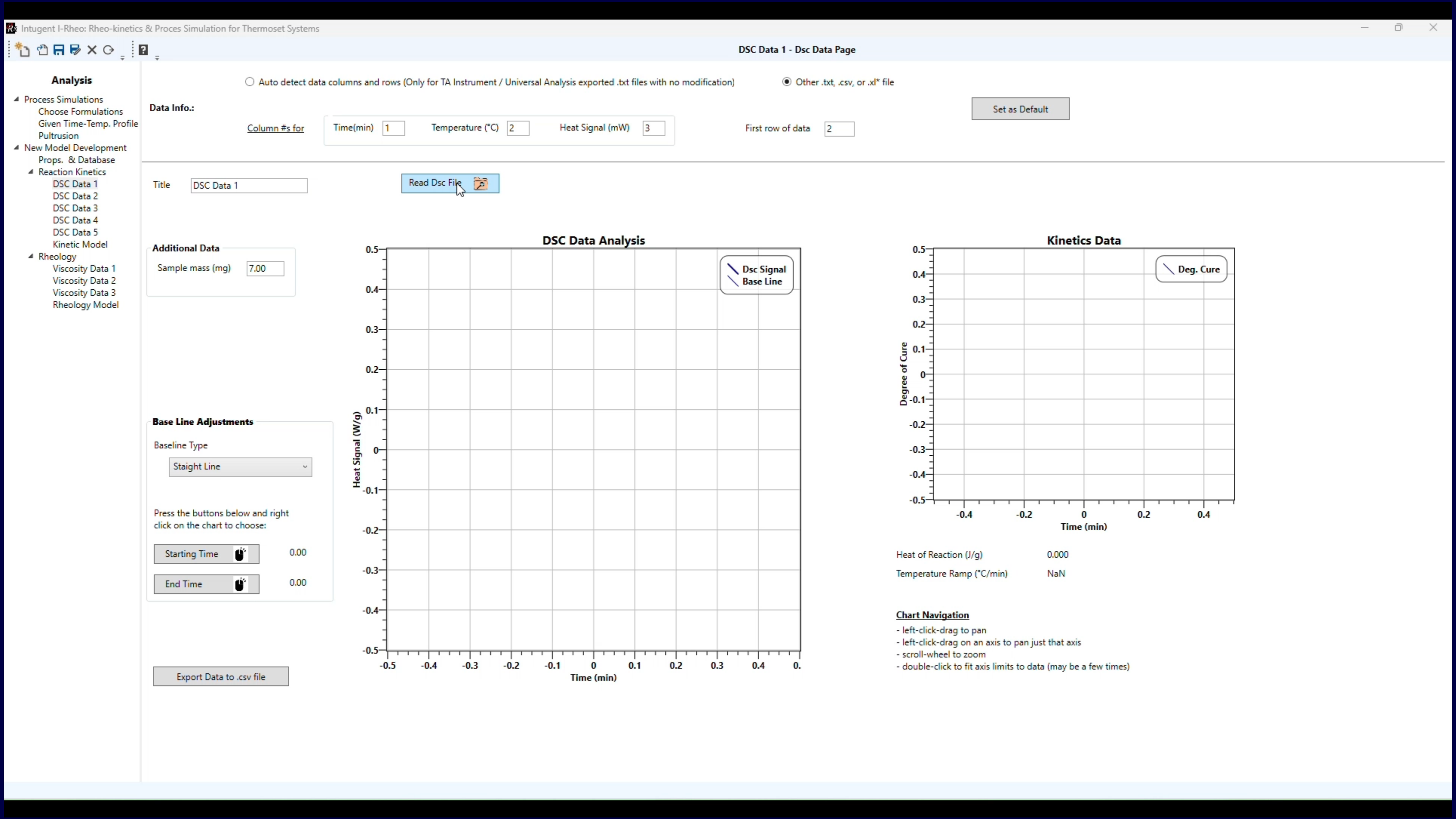
Seferis Model

$$\eta = \eta_0 \, exp\left(\frac{E_\eta}{\Re T}\right) \; exp(K_s \alpha)$$

WLF Model

$$\eta \; = \eta_0 \, exp\left(\frac{-\,\boldsymbol{C_1}\,(\boldsymbol{T}-\boldsymbol{T_g})}{\boldsymbol{C_2} + (\boldsymbol{T}-\boldsymbol{T_g})}\right)$$

Developing Rheokinetic Model with I-Rheo

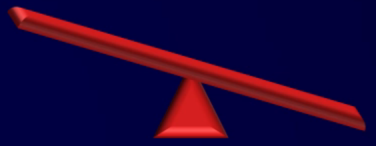


Filament Winding & Pultrusion with I-Rheo

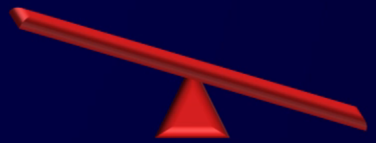
Filament Winding

- Relatively slow process
- Time-temperature profile is know with fair certainty
- Use Rheokinetic Simulation with given time-temperature profile module

- Initial Viscosity: resin uptake



- Minimum Viscosity: Wetting



- Optimize time-temperature profile to improve productivity

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Conclusions

- Digital Transformation can help in improving quality and speed of innovations
- Digital Transformation Software are available that provide digital platform for new innovations and process improvements
- Engineer and Researchers do not need to have any background in AI, Finite Elements, and math modeling to leverage these tools
- AI and sAI models with user friendly interface can be used to predict the final properties
- Process scaleup models allow engineers to simulate industrial scale applications

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