CANFSA
Center for Advanced
Non-Ferrous Structural Alloys
An Industry/University Cooperative Research Center

"New" thoughts and work on ML/AI

Rigorously relating physics with ML/AI

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My point of view:
(hopefully disarming to the rationally doubtful)

#1). Machine learning / artificial intelligence is powerful, and therefore widely pursued with a great many papers being published…

…but, often, it is adopted without thought, and the number of papers does not relate to the quality of the work, but the popularity and "citability" of the topic. This is enormously risky!!

#2). They can be used for a variety of problems: recognition/classification, correlation, simulation of 'fakes', …

…but let us simplify and say they all seek to correlate Xi's with Y's, even if Xi's are rarely presented

#3). The 'promise' is that ML/AI will provide us great new insights and permit challenging problems to be "automatically solved"…

…but new insights are only helpful if we can interpret them and <u>extrapolate</u> beyond our training sets for new problems…

…and, there is nothing "automatic" about <u>most</u> good ML/AI work

#4). We know many of the physics of many of our problems, and there is a gulf between ML/AI and our fundamental physics…

…but this is simply a problem that hasn't been solved

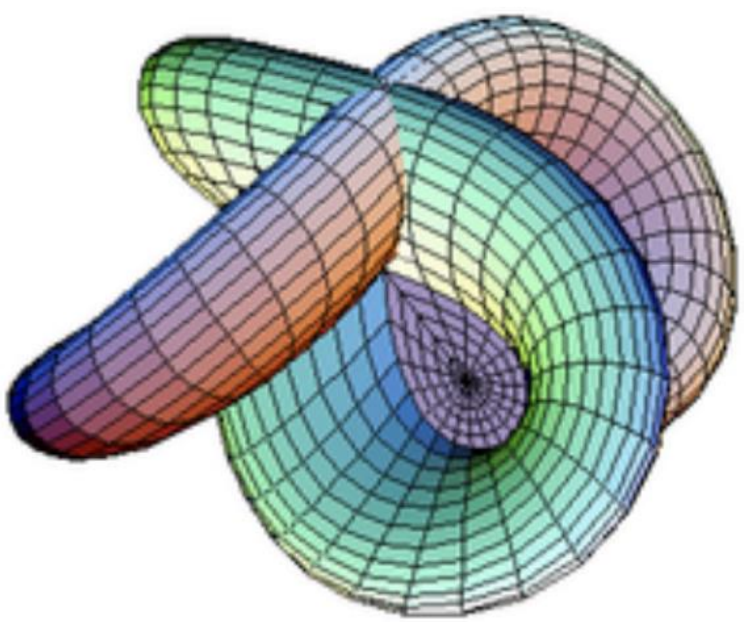
Some background:

A few words on ML/AI

Fundamentally, ML/AI techniques seek to correlate (map) inputs with outputs.

The easiest way to 'accurately' imagine ML/AI is to consider a N-variable manifold (hypersurface).

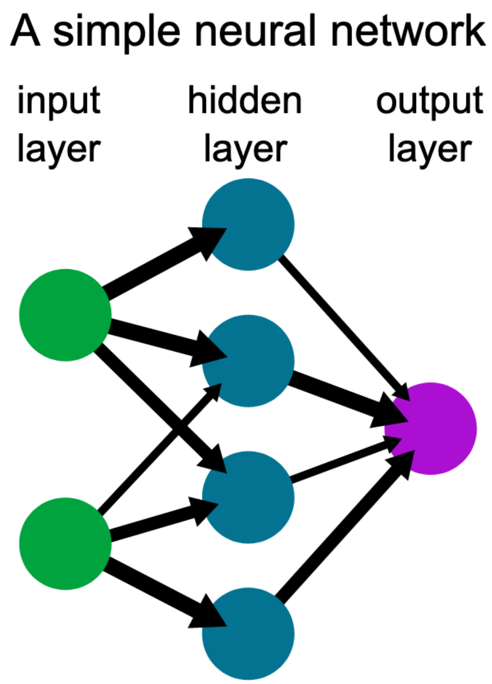
The underlying basis vectors are the input variables (Xi's) that affect the output Y, and the hypersurface is a map of Y for all Xi's.

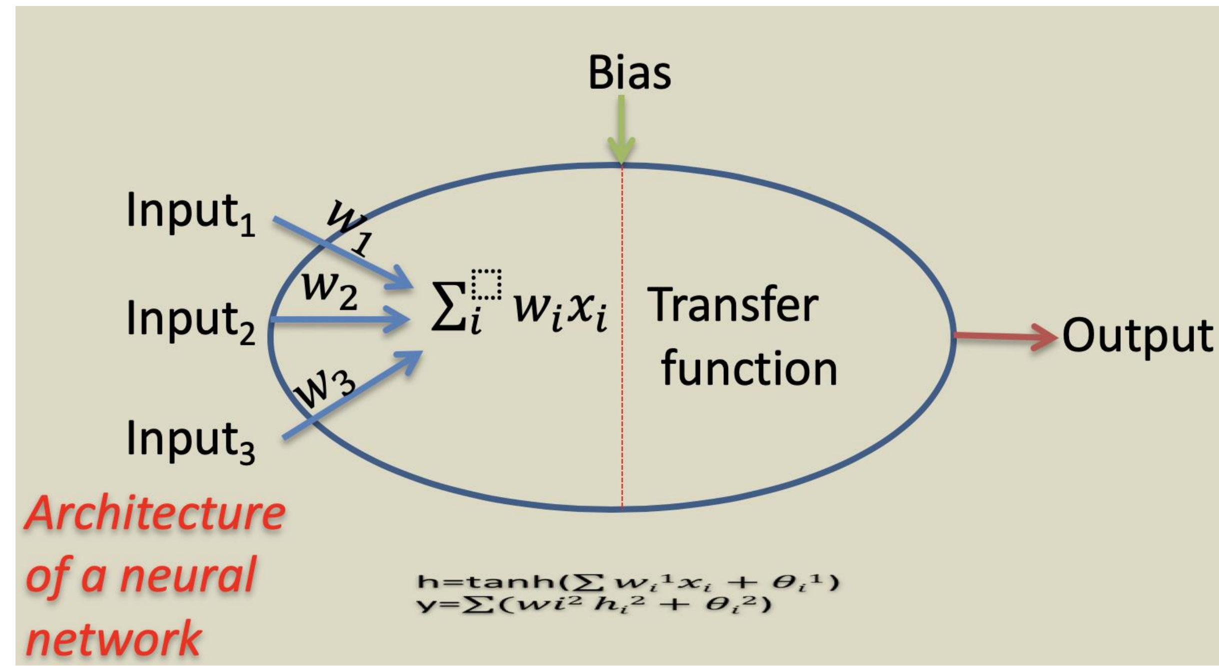


Some consequences:
Locally 'flat', meaning that similar sets of Xi's will give similar Y.
(underpins various networks, including those focused on classification, ANNs, GANs, etc)

Typically relies upon flexible mathematical equations.

A bit more background:





Neural networks use very flexible functions (e.g., tanh, ReLU, Softmax, Logistic Sigmoid, Standardization, …), and architect them using weights, biases, and summations…

An unusual way of thinking of these: You can think that these functions modify the underlying data until the summation gives an output with acceptable performance.

In other words, these functions perform affine transforms on the data…until it approaches/approximates the manifold/hypersurface/hull

About 10 years ago, we asked: Is it not possible that two equations represent the same 'response surface'

Some prior work:

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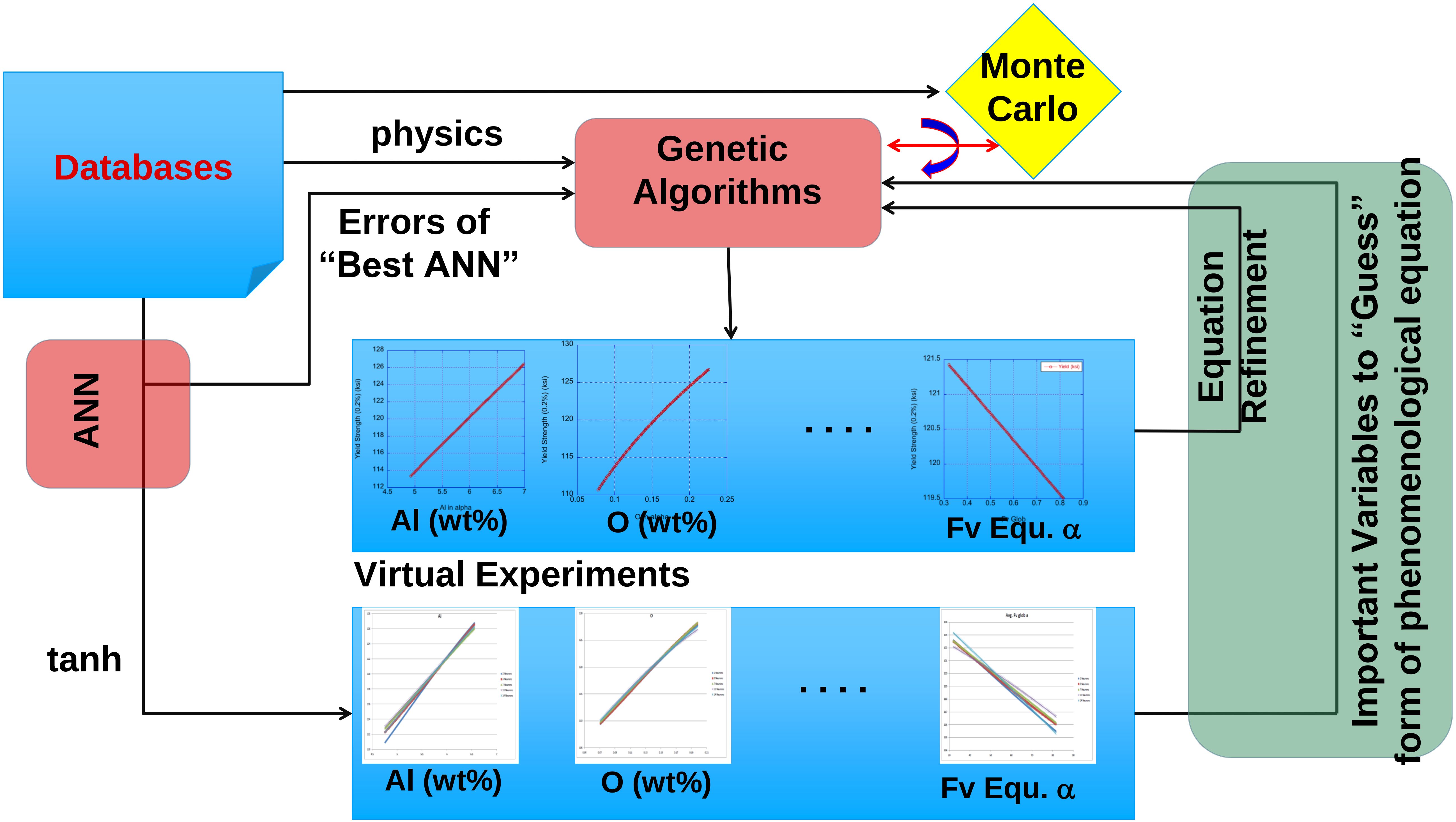
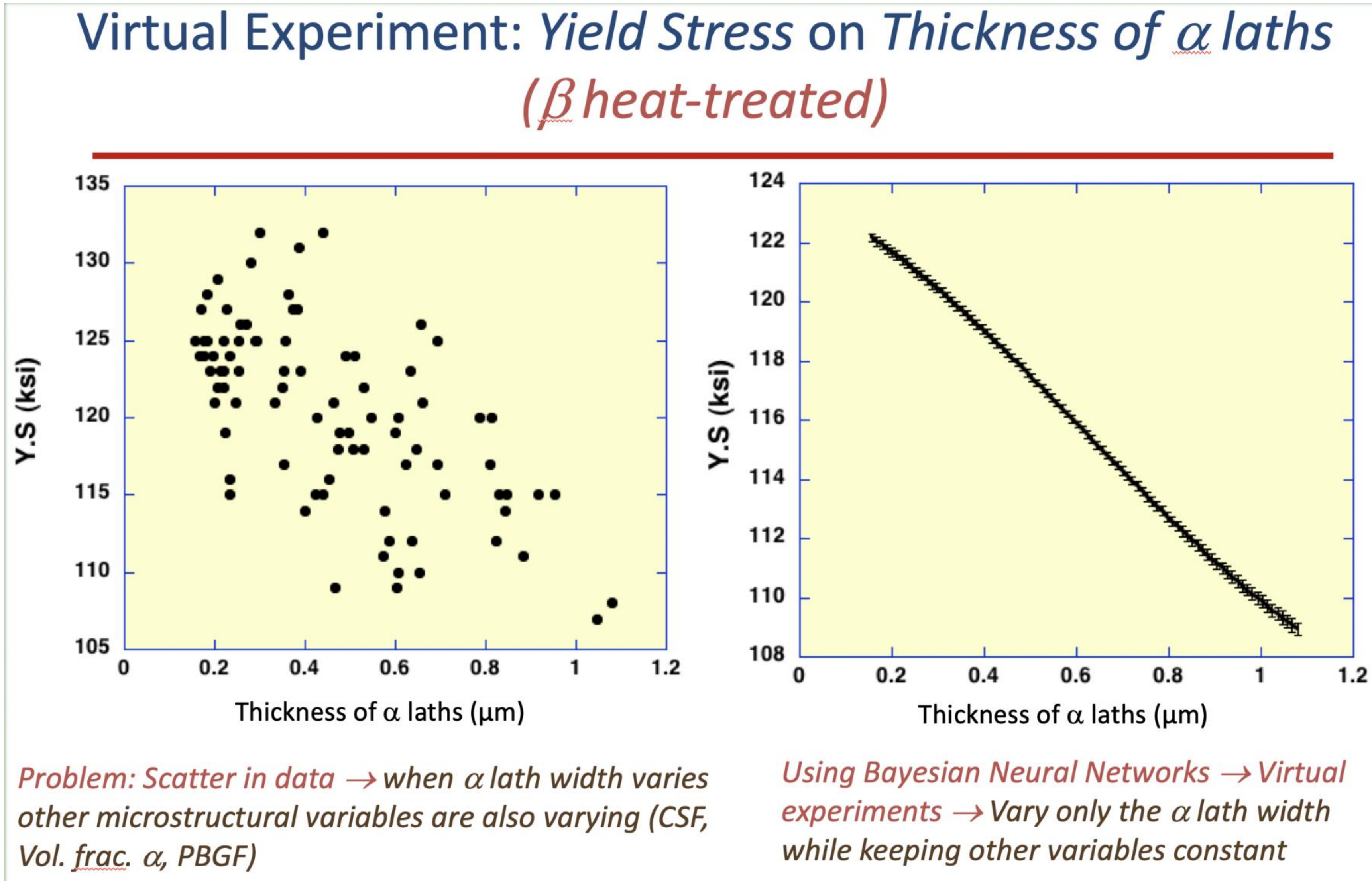


Some prior work:



Avoid overfitting: risk of obtaining higher order manifolds than necessary (this harkens to statistics, error, and perceptrons)

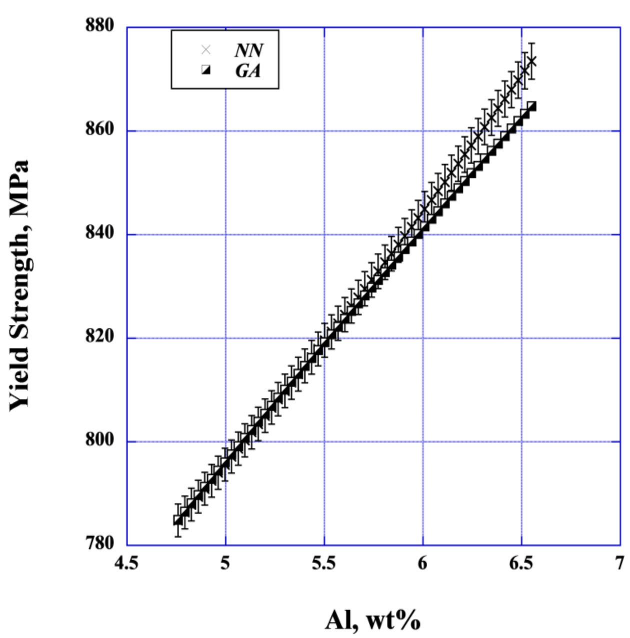
Some prior work:

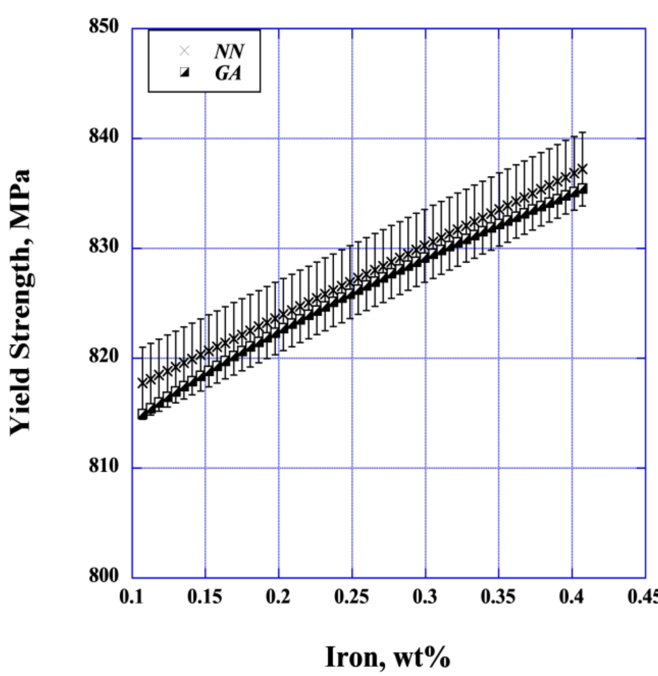
GA-derived phenomenological equation

$$\boxed{\sigma_{ys}} = \boxed{\sigma_o} + \sigma_{ss} + \boxed{\sigma_{grainsize}} + \boxed{\sigma_{interface}}$$

22 unknowns!!!

$$Yield(MPa) = \boxed{(b_1 * F_V^{\alpha}) + (b_2 * (1 - F_V^{\alpha}))} + \boxed{F_V^{\alpha} * (b_3 * C_{Al}^{n_{Al}} + b_4 * C_O^{n_O})} +$$
$$\boxed{(1 - F_V^{\alpha}) * ((b_5 * C_V^{n_V})^{n_1} + (b_6 * C_{Fe}^{n_{Fe}})^{n_2})^{n_3}} + \boxed{b_7 * F_V^{Equiaxed\_\alpha} * Equiaxedsize^{-n_4}} +$$
$$(1 - F_V^{Equiaxed\_\alpha}) * (C + \boxed{b_8 * \frac{\frac{Equiaxedsize}{F_V^{Equiaxed\_\alpha}} - Equiaxedsize}{Lathwidth}} + b_9 * (\frac{Equiaxedsize}{F_V^{Equiaxed\_\alpha}} - Equiaxedsize)^{-n_5}) +$$
$$\boxed{b_{10} * \frac{(F_V^{\alpha} - F_V^{Equiaxed\_\alpha}) * lathwidth - MIN}{MAX - MIN}} * (1 - F_V^{\alpha}) + b_{11} * (Lathwidth)^{-n_6}$$





$$\sigma_{ys} = \sigma_o + \sigma_{ss} + \sigma_{grainsize} + \sigma_{interface}$$

$$Yield(MPa) = (88.5 * F_V^{\alpha}) + (63 * (1 - F_V^{\alpha})) + F_V^{\alpha} * (148.5 * C_{Al}^{0.63} + 724.5 * C_O^{0.6}) +$$
$$(1 - F_V^{\alpha}) * ((49.8 * C_V^{0.63})^{0.45} + (240 * C_{Fe}^{0.82})^{0.48})^{2.12} + 0.02 * F_V^{Equiaxxed\_\alpha} * Equiaxedsize^{-0.33} +$$
$$(1 - F_V^{Equiaxed\_\alpha}) * (154 + 0.15 * \frac{\frac{Equiaxedsize}{F_V^{Equiaxed\_\alpha}} - Equiaxedsize}{Lathwidth} + 0.01 * (\frac{Equiaxedsize}{F_V^{Equiaxed\_\alpha}} - Equiaxedsize)^{-0.32}) +$$
$$18.5 * \frac{(F_V^{\alpha} - F_V^{Equiaxed\_\alpha}) * lathwidth - MIN}{MAX - MIN} * (1 - F_V^{\alpha}) + 0.015 * (Lathwidth)^{-0.53}$$

- σ_0^{α}=78.4 to 90MPa (well-annealed) Anderson, E.A., D.C. Jillson, and S.R. Dunbar, AIME Trans. , 1953. **197**: p. 1191-7
  Predicted σ_0^{α} is 88.5 MPa
- $\sigma_0^{\beta} < \sigma_0^{\alpha}$ (α has 3 slip systems while β has at least 12 slip systems)
  Predicted σ_0^{β} is 63
- Influence of elements on the yield strength O>Fe>Al>V
  A_O=724.5; A_{Fe}=240; A_{Al}=148.5; A_V=49.8
  "A" value is a function of the difference in shear modulus and size

Ankem, S., G. K. Scarr, et al. (1988). Multiple regression analysis of the effects of various alloying elements on the properties of titanium alloys. Sixth world conference on titanium, France

Collins, P. C., S. Koduri, et al. (2012). "Neural networks relating alloy composition, microstructure and tensile properties of a/b processed TIMETAL 6-4." Metallurgical and materials transaction A.

G_{Ti}=44GPa	r_{Ti}=0.140nm
G_V=47 GPa	r_V=0.132 nm
G_{Fe}=82 GPa	r_{Fe}=0.126 nm

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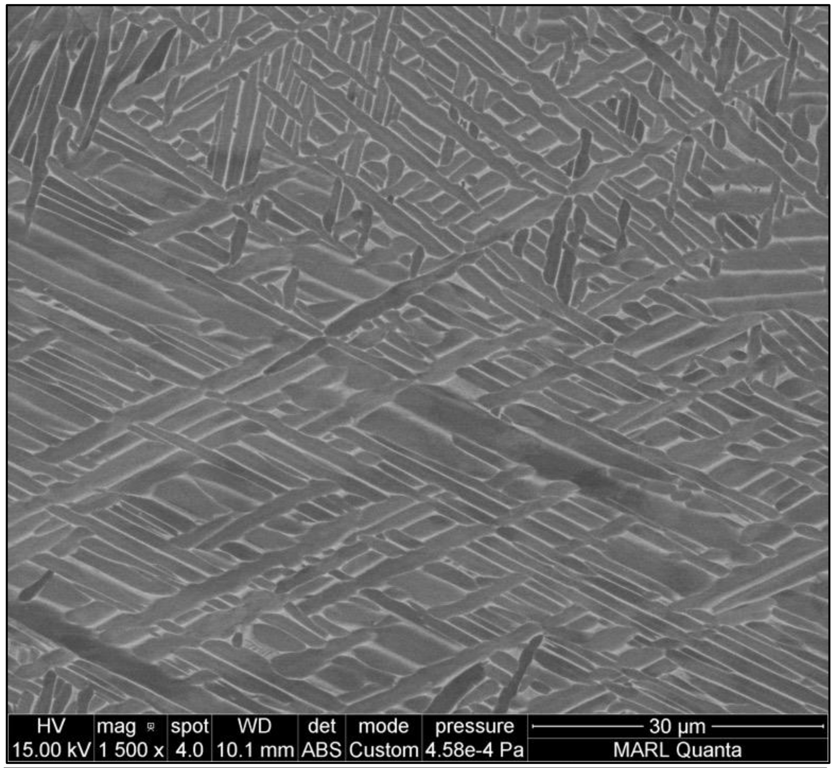
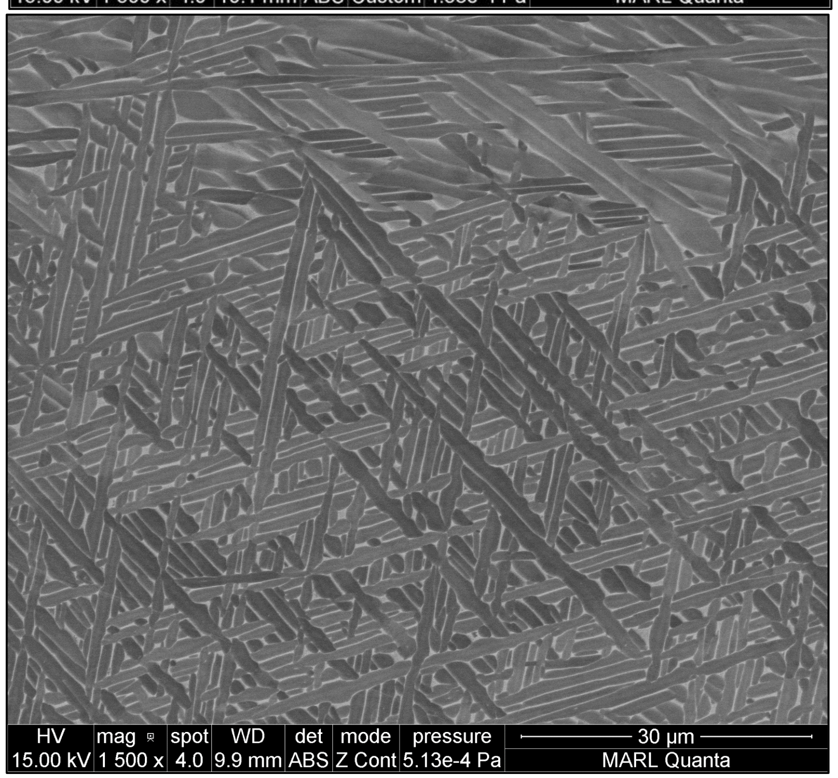
Some current work:





$$\sigma_{ys} = \begin{cases} F_V^{\alpha}\cdot\sigma_O^{\alpha} + F_V^{\beta}\cdot\sigma_O^{\beta} + & \text{Intrinsic Strength} \\ F_V^{\alpha}\cdot\sigma_{SS}^{\alpha} + F_V^{\beta}\cdot\sigma_{SS}^{\beta} + & \text{Solid Solution Strengthening} \\ F_V^{col}\cdot C_{\alpha-lath}\cdot(t_{\alpha-lath})^{n}\cdot(t_{\beta-rib})^{-n} + & \text{Hall -- Petch Strengthening (alpha laths)} \\ F_V^{col}\cdot C_{col}\cdot(t_{colony})^{n} + & \text{Hall -- Petch Strengthening (colonies)} \\ (-1)\cdot(AxisDebit) + & \text{Texture Debits (easier slip)} \\ F_V^{BW}\cdot\alpha MGb\sqrt{\rho} & \text{Taylor Hardening} \end{cases} \qquad (2)$$

$$\sigma_{ys} = \begin{cases} F_V^{\alpha}\cdot 89 + F_V^{\beta}\cdot 45 + \\ F_V^{\alpha}\cdot\left(149\cdot x_{Al}^{0.667} + 759\cdot x_O^{0.667}\right) + F_V^{\beta}\cdot\left(\left(22\cdot x_V^{0.7}\right)^{0.5} + \left(235\cdot x_{Fe}^{0.7}\right)^{0.5}\right)^2 \\ + \\ F_V^{col}\cdot 150\cdot(t_{\alpha-lath})^{-0.5}\cdot(t_{\beta-rib})^{0.5} + \\ F_V^{col}\cdot 125\cdot(t_{colony})^{-0.5} + \\ (-1)\cdot(AxisDebit) + \\ F_V^{BW}\cdot\alpha MGb\sqrt{\rho} \end{cases} \qquad (3)$$

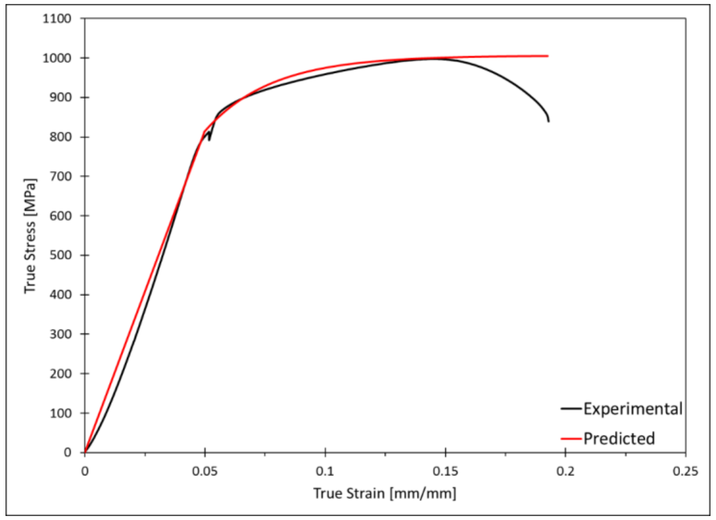
Sample ID	Fv alpha	CoV Fv alpha	a-lath width (m)	CoV a-lath width	% Colony (est)
A05	87.51	0.039	0.388	0.146	10
A06	88.93	0.004	0.392	0.074	30
A07	91.83	0.014	0.483	0.1	20

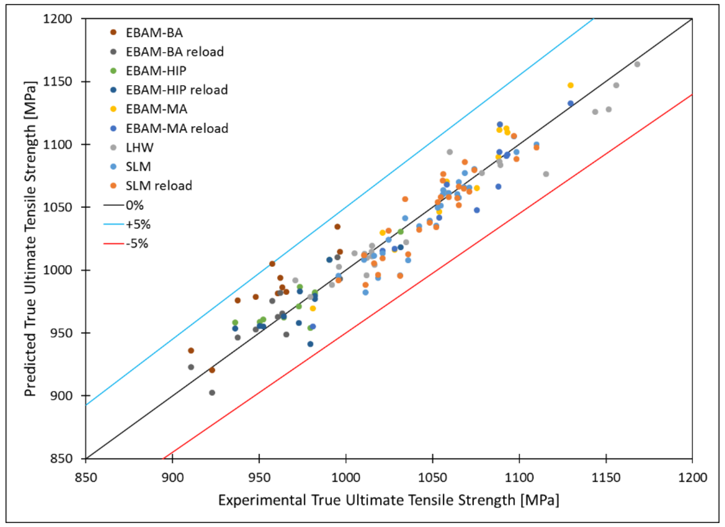
Sample ID	Ti wt%	Al wt%	V wt%	Ti at%	Al at%	V at%
A05	90.27	6.29	3.44	86.24	10.67	3.09
A06	90.28	6.37	3.36	86.2	10.79	3.01
A07	90.22	6.3	3.47	86.19	10.69	3.12

Sample ID	Pred. YS	Meas. YS	Pred. UTS***	Meas UTS
A05	116.7	115.7	132.2	131.5
A06	120.9	122.3	135	141.8
A07	120.7	119.8	135	134.3

$$\sigma = \sigma_0 + \frac{\alpha GMbk_1}{k_2}\left(1-\exp\left(-\frac{k_2M\varepsilon}{2}\right)\right)$$

$$\varepsilon_{n-KM} = \frac{2}{k_2M}\ln\left(\frac{(2+k_2M)(\alpha GbMk_1)}{2(\alpha GbMk_1 + k_2\sigma_0)}\right)$$





A single equation: wrought, 3 variants of AM, + HTs

Returning to My point of view:

#3). The ‘promise’ is that ML/AI will provide us great new insights and permit challenging problems to be “automatically solved”…

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…and, there is nothing “automatic” about <u>most</u> good ML/AI work

#4). We know many of the physics of many of our problems, and there is a gulf between ML/AI and our fundamental physics…

…but this is simply a problem that hasn’t been solved

Revisiting our hypothesis: Is it not possible that two equations represent the same ‘response surface’

Surely an expansion would work – perhaps Taylor series??

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Returning to my point of view:

Science AAAS

Submitted Manuscript: Confidential

A General Approach for Learning Constitutive Relationships (Physical Laws) from Neural Networks

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Abstract: This paper presents a new theorem by which physical phenomenon and their associated laws and theories can be learned from highly flexible mathematical functions exploited in neural networks. We provide a methodology in which formulae of both hypothesized physical mechanisms and neural networks can be re-expressed using their Fourier series expansions. By invoking the uniqueness theorem, the coefficients of the Fourier series expansions of the basis functions of the neural networks are shown to correspond to those of physical phenomena, enabling the structure of a neural network for a data corpus to be rewritten into their physicum operandi – or vice versa. This approach not only provides new interpretability to a variety of machine learning/artificial intelligence approaches, but also permits known physical information to pre-structure those methods.

$$b_m = \sum_{k=-\infty}^{\infty} c_k \sum_{q=0}^{\infty} \frac{(2\pi i k)^q}{q!} \sum_{\substack{\sum_{j\in\mathbb{Z}} q_j = q \\ \sum_{j\in\mathbb{Z}} j q_j = m}} \binom{q}{\dots, q_{-j}, \dots, q_j, \dots} \prod_{n\in\mathbb{Z}} a_n^{q_n}.$$

$$f_{NN}(x) - f_{CR}(x) = \sum_{k=-\infty}^{\infty} a_k e^{2\pi i k x} - b_k e^{2\pi i k x} = 0 \leftrightarrow a_k = b_k \forall k.$$

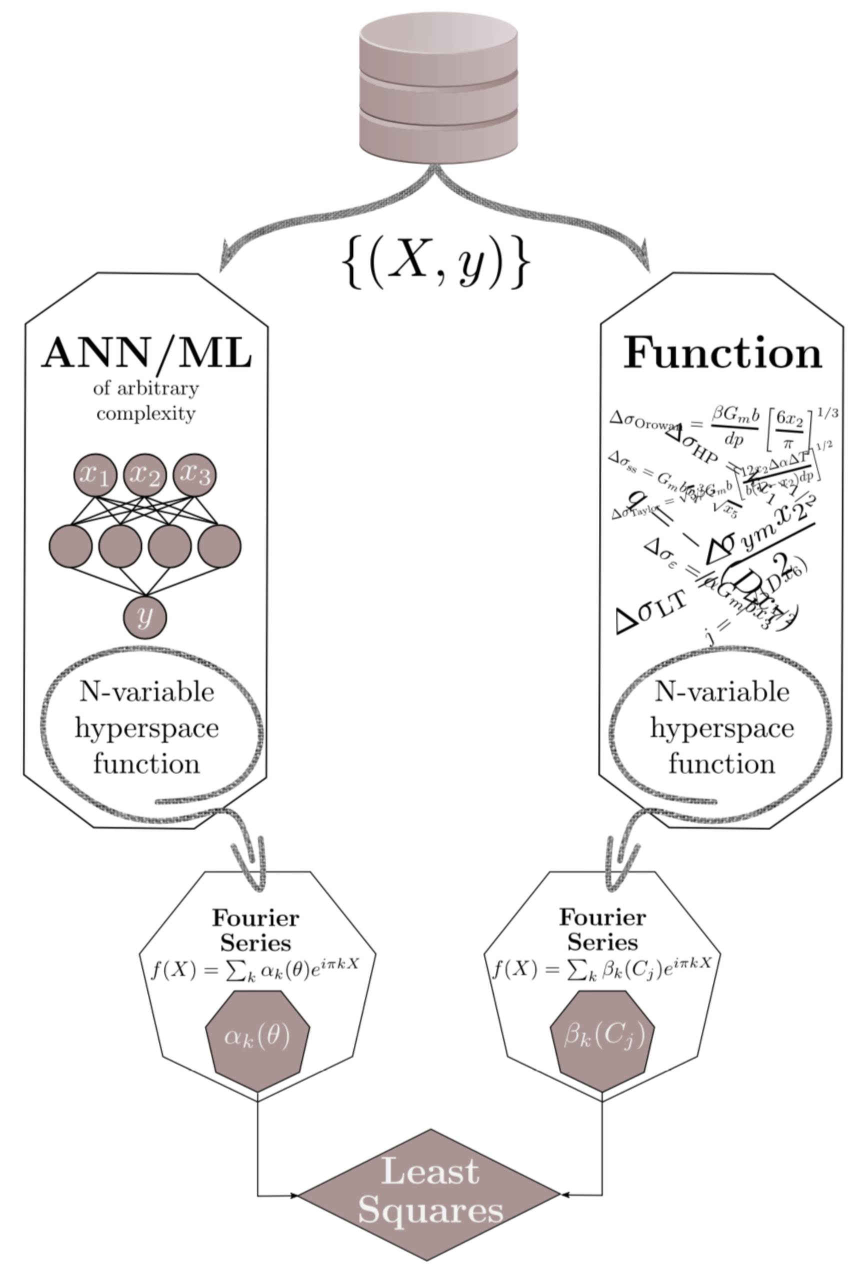

Figure 1. Schematic showing the construction of an ML model (left branch) and a candidate constitutive relationships (right branch), each expanded on a Fourier basis set. Since both are supported by the same basis, the Fourier coefficients of the two expansions are directly comparable.

Outcomes

We were wrong on Taylor series expansion – the radius of convergence collapses to zero, and it doesn't work.

It is necessary to have a series with a non-vanishing radius of convergence – a property of the Fourier series expansion

THIS WORKS (and we have proven so – we think)

Physical phenomena are absolutely and directly interpretable from ML/AI

Only the NN architecture and activation functions are required to determine a functional relationship – in other words, once solved once, this is a fast process.

Physics can *preseed* NNs

    If some physics are known, some physics can preseed 'classes' of architectures

This overcomes the main barriers of ML/AI:

extrapolation vs. interpolation and no connection to fundamental science/knowledge

Additional Outcomes

We have developed the maths for accuracy/error.

The problem is currently ugly, but a candidate for supercomputing and arguably quantum

We have started to sort out candidate functions

Other functions (including time dependent phenomenon) should be possible

Table 1. Common activation functions for neural networks.

Name	$f(x) =$	c_k
Softmax	$\frac{e^{x_j}}{\mathbb{Z}}, \mathbb{Z} = \sum_{n=1}^{N} e^{x_n}$	$\frac{1}{\mathbb{Z}} \frac{(e^L - 1)}{L - 2\pi \mathbb{i} k}$
ReLU	$\begin{cases} x, & x \geq 0 \\ 0, & x < 0 \end{cases}$	$\begin{cases} \frac{\mathbb{i} L}{2\pi k}, & k \neq 0 \\ \frac{L}{2}, & k = 0 \end{cases}$ for $x > 0$
Logistic Sigmoid	$\frac{1}{1 + e^{-x}}$	Undefined
Standardization	$\frac{x}{\sigma} - \frac{\mu}{\sigma}$	$\frac{\mathbb{i} L}{2\pi k \sigma}$

Table 2. Example constitutive functions and their Fourier coefficient generating functions. $\ln x$, the natural logarithm; $C(x) = \int_0^x \cos t^2 \, dt$, the Fresnel Cosine Integral; $S(x) = \int_0^x \sin t^2 \, dt$, the Fresnel Sine Integral; $E_n(x) = \int_1^\infty e^{-x\,t}/t^n dt$, the Exponential Integral; and $\Gamma(x, a) = \int_a^\infty t^{x-1} e^{-t} dt$, the Incomplete Gamma Function.

$f(x) =$	c_k
$A\alpha^x$	$\frac{(\alpha^L - 1)A}{L \ln \alpha - 2\pi \mathbb{i} k}$
$Ax^\alpha, \alpha > 0$	$\frac{A\, L^\alpha}{(2\pi \mathbb{i} k)^{1+\alpha}} [\Gamma(1+\alpha) - \Gamma(1+\alpha, 2\pi \mathbb{i} k)]$
$Ae^{-\alpha\, x}$	$\frac{A(1 - e^{-\alpha L})}{\alpha L + 2\pi \mathbb{i} k}$
$\frac{A}{\sqrt{x}}$	$\frac{A\left[C\left(2\sqrt{k}\right) - \mathbb{i}\, S\left(2\sqrt{k}\right)\right]}{\sqrt{kL}}$
$A\,(1+x)^\alpha$	$\frac{A}{L}\, e^{\frac{2\pi \mathbb{i} k}{L}} \left[E_{-\alpha}\left(\frac{2\pi \mathbb{i} k}{L}\right) - (1+L)^{1+\alpha} E_{-\alpha}\left(2\pi \mathbb{i} k \frac{1+L}{L}\right)\right]$
$A\,log(1+x)$	$\frac{A\left[e^{2\pi \mathbb{i} k/L}\left[\Gamma\left(0, \frac{2\pi \mathbb{i} k}{L}\right) - \Gamma\left(0, \frac{2\pi \mathbb{i}(1+L)}{L}\right)\right] - \log(1+L)\right]}{2\pi \mathbb{i} k}$

Closing thoughts

Two methods, both alike in dignity,
In fair sciences, where we lay our scene.
From ancient elegance break to methods mutinous,
Where machine learning makes physical laws unclean,
From forth the noble loins of these two foes
A pair of cross-term'd numbers seek their place;

Whose serial expansions, equally covariant
Do with their projections, bury their parents strife.
Our fearful assessment of their dual-space truth,
And the continuance of their parents, sage,
Which, for their children's union, sought to achieve,
Is now the two hours' traffic of our stage;

The which, if you with patent eyes attend,
What here shall miss, our toil shall strive to mend.