

A GENERAL APPROACH FOR LEARNING CONSTITUTIVE RELATIONSHIPS (PHYSICAL LAWS) FROM NEURAL NETWORKS

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1. METHODS

Fully dense neural network (NN) architectures, such as the one shown in Figure 1, perform a sequence of affine transformations, $\mathbf{z}_i \leftarrow \boldsymbol{\theta}_i \mathbf{x}^{(i)}$, followed by element-wise functional operations, $\sigma(\mathbf{z}_i)$ to introduce non-linearity at each layer; that is, each layer stretches and distorts the underlying space.

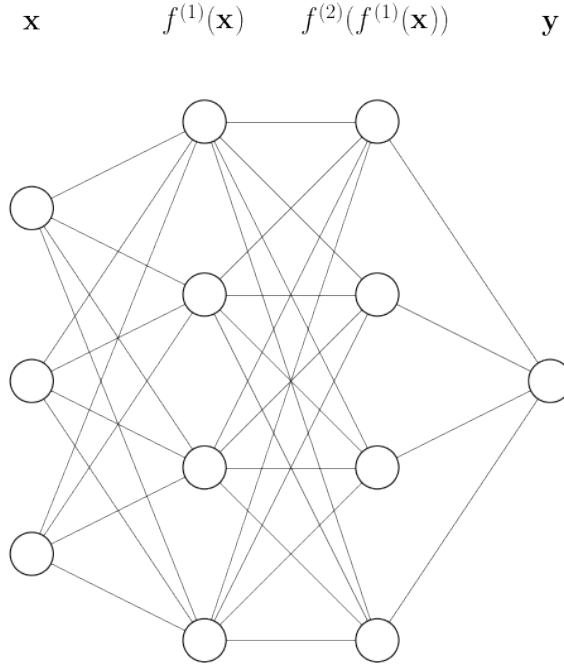


FIGURE 1. Schematic view of a fully dense neural network. Each sequence of affine and non-linear transformations are captured in the function, $f_i(\mathbf{x}) : \mathbf{x}^{(i+1)} \leftarrow \sigma(\boldsymbol{\theta}_i \mathbf{x}^{(i)})$

The resulting network,

$$(1) \quad f(x) = \sigma(\theta_n \sigma(\theta_{n-1} \sigma(\dots \theta_2 \sigma(\theta_1 x))))$$

is an arbitrary function generator, but at present, the network weights θ_i can not map back to analytic forms that capture and describe the underlying physics. There are, however, many such mappings through polynomial series expansions,

$$(2) \quad f(x) = \sum_{n=0}^{\infty} a_n x^n$$

We hypothesize that the physics of a process can be extracted by fitting the polynomial expansions of known physical relationships to the polynomial coefficients of a polynomial series expansion of Equation (1).

Although ReLU (rectified linear units) have become a more common activation function, its discontinuity at $x = 0$ requires an infinite series to fully capture the behavior at this transition. However, the sigmoid function,

$$(3) \quad \sigma(x) = \frac{1}{1 + e^{-x}}$$

is a special case of the generating function for the Euler polynomial coefficients,

$$(4) \quad \frac{2e^{xt}}{1 + e^t} = \sum_{n=0}^{\infty} E_n(x) \frac{t^n}{n!}$$

where, for $x = 0$,

$$(5) \quad \sigma(x) = \frac{1}{2} \sum_{n=0}^{\infty} E_n(0) \frac{(-1)^n}{n!}.$$

The Euler polynomials at $x = 0$,

$$(6) \quad E_n(0) = -2(n+1)^{-1} (2^{n+1} - 1) B_{n+1}$$

where B_n is the n^{th} Bernoulli number. Since Bernoulli numbers of odd index, with the exception of B_1 , are zero, $E_i(0) = 0$ for $i = 2, 4, 6, \dots, 2n$. Therefore, the summand and limits of Equation (5) change to

$$(7) \quad \sigma(x) = \frac{1}{2} - \frac{1}{2} \sum_{n=1}^{\infty} \left(\frac{E_{2n-1}(0)}{(2n-1)!} \right) x^{2n-1}.$$

The series representation of $E_{2n-1}(x)$

$$(8) \quad E_{2n-1}(x) = \frac{(-1)^n 4(2n-1)!}{\pi^{2n+1}} \sum_{k=0}^{\infty} \frac{\cos[(2k+1)\pi x]}{(2k+1)^{2n}}$$

such that,

$$(9) \quad E_{2n-1}(0) = \frac{(-1)^n 4(2n-1)!}{\pi^{2n+1}} \sum_{k=0}^{\infty} \frac{1}{(2k+1)^{2n}}$$

and therefore,

$$\begin{aligned}
 (10) \quad \sigma(x) &= \frac{1}{2} - \sum_{n=1}^{\infty} 2 \frac{(-1)^n}{\pi^{2n}} \left(\sum_{k=0}^{\infty} \frac{1}{(2k+1)^{2n}} \right) x^{2n-1} \\
 &= \frac{1}{2} - \sum_{n=1}^{\infty} 2 \frac{(-1)^n}{\pi^{2n}} (4^{-n} (4^n - 1) \zeta(2n)) x^{2n-1} \\
 &= \frac{1}{2} - \sum_{n=1}^{\infty} 2 \underbrace{\left(\frac{-1}{4\pi^2} \right)^n (4^n - 1) \zeta(2n)}_{a_n} x^{2n-1} \\
 (11) \quad &= \sum_{n=0}^{\infty} a_n x^n, \quad a_n = \begin{cases} 1/2 & n = 0 \\ -2 \left(\frac{-1}{4\pi^2} \right)^{(n+1)/2} (4^{(n+1)/2} - 1) \zeta(n+1) & n \text{ odd} \\ 0 & n \text{ even} \end{cases}
 \end{aligned}$$

2. DISCUSSION

Many non-trivial problems in materials science, and in science more broadly, are explained not through a single constitutive relationship, but through a superposition of contributing physics.

Figure ?? shows an artificial dataset constructed to replicate the impact of yield stress in a two-phase, solid-solution strengthened alloy system. Using a combination of composite theory for the contribution of flow stress, **NAME** solid solution [?], and Hall-Petch [?] strengthening, the expected yield stress is

$$(12) \quad \sigma_y = F_v^A \sigma_f^A + F_v^B \sigma_f^B + \sum_i C_i [x_i]^{2/3} + \sum_j k_j d_j^{-1/2} + \dots$$

with free parameters

- F_v^i Volume fraction of phase i
- $[x_i]$ Concentration of solute i
- d_j Average grain diameter of phase j

and fixed parameters

- σ_f^i Flow stress of phase i
- C_i Solid solution strengthening coefficient for solute species i
- k_j Hall-Petch strengthening coefficient for phase j

The goal is to iteratively improve on this constitutive model one term at a time, and monitor the effect on the residuals between the predicted yield, $\hat{\sigma}_y$ and the actual yield σ_y .

The analytical form, combining Equations (1) and (11), the estimated output of a two-layer NN can be written as

$$\begin{aligned}
 \mathbf{y}_1 &= \sum_{k=0}^{\infty} a_k (\boldsymbol{\theta}_1^T \mathbf{x})^k \\
 \mathbf{y}_2 &= \sum_{k=0}^{\infty} b_k (\boldsymbol{\theta}_2^T \mathbf{y}_1)^k \\
 &= b_0 \mathbf{1} + \\
 &\quad + b_1 (\tilde{a}_0 + (\tilde{a}_1 + (\tilde{a}_2 + (\tilde{a}_3 + (\dots) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \\
 &\quad + b_2 (\tilde{a}_0 + (\tilde{a}_1 + (\tilde{a}_2 + (\tilde{a}_3 + (\dots) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \tilde{\mathbf{x}})^2 \\
 &\quad \vdots \\
 &\quad + b_k (\tilde{a}_0 + (\tilde{a}_1 + (\tilde{a}_2 + (\tilde{a}_3 + (\dots) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \tilde{\mathbf{x}}) \tilde{\mathbf{x}})^k \\
 &\quad \vdots \\
 &\quad \text{where } \tilde{a}_i = \boldsymbol{\theta}_2^T a_i, \tilde{\mathbf{x}} = \boldsymbol{\theta}_1^T \mathbf{x} \\
 (13) \quad &= \sum_{N=0}^{\infty} b_N \sum_{j=0}^N \binom{N}{j} \tilde{a}_0^{N-j} \sum_{k=0}^j \binom{j}{k} \tilde{a}_1^{j-k} \dots \tilde{\mathbf{x}}^{j+k+\dots} \\
 &= \sum_{N=0}^{\infty} \sum_{j=0}^N \sum_{k=0}^j \dots b_N \binom{N}{j} (\boldsymbol{\theta}_2^T a_0)^{N-j} \binom{j}{k} (\boldsymbol{\theta}_2^T a_1)^{j-k} \dots (\boldsymbol{\theta}_1^T \mathbf{x})^{j+k+\dots} \\
 &= \sum_{N=0}^{\infty} \sum_{j=0}^N \sum_{k=0}^j \dots b_N \binom{N}{j} \binom{j}{k} \dots (\boldsymbol{\theta}_2^T a_0)^{N-j} (\boldsymbol{\theta}_2^T a_1)^{j-k} \dots (\boldsymbol{\theta}_1^T \mathbf{x})^{j+k+\dots} \\
 (14) \quad &= \sum_{k=0}^{\infty} c_k (\boldsymbol{\theta}_1^T \mathbf{x})^k
 \end{aligned}$$

If $a_i = 0 \forall i$ even, then are Equations (13-14) everywhere 0?
 How does dropout affect this?