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.

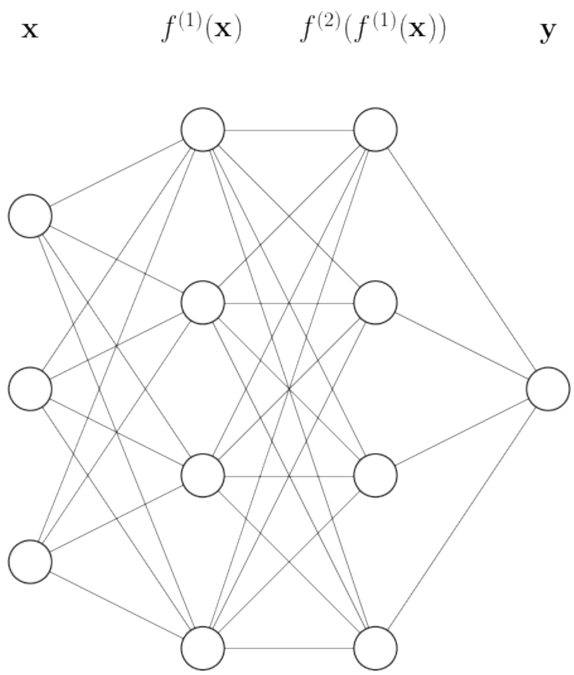

Figure 1. Schematic view of a fully dense neural network. Each sequence of affine and non-linear transformations are captured in the function, $f_i(\mathbf{x})$: $\mathbf{x}^{(i+1)} \leftarrow \sigma(\boldsymbol{\theta}_i \mathbf{x}^{(i)})$

The resulting network,

$$f(x) = \sigma(\boldsymbol{\theta}_n \sigma(\boldsymbol{\theta}_{n-1} \sigma(\ldots \boldsymbol{\theta}_2 \sigma(\boldsymbol{\theta}_1 \mathbf{x})))) \tag{1}$$

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

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

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,

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

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

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

where, for $x = 0$,

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

The Euler polynomials at $x = 0$,

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

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 $i = 2, 4, 6, \ldots, 2n$. Therefore, the summand and limits of Equation (5) change to

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

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

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

such that,

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

and therefore,

$$\begin{aligned}
\sigma(x) &= \frac{1}{2} - 2\sum_{n=1}^{\infty} \frac{(-1)^n}{\pi^{2n}} \left(\sum_{k=0}^{\infty} \frac{1}{(2k+1)^{2n}} \right) x^{2n-1} && (10) \\
&= \frac{1}{2} - 2\sum_{n=1}^{\infty} \frac{(-1)^n}{\pi^{2n}} \left(4^{-n} \left(4^n - 1\right) \zeta(2n) \right) x^{2n-1} \\
&= \frac{1}{2} - 2\sum_{n=1}^{\infty} \left(\frac{-1}{4\pi^2} \right)^n \left(4^n - 1\right) \zeta(2n) x^{2n-1} \\
&= \frac{1}{2} - 2\sum_{n=1}^{\infty} a_n x^{2n-1}, \; a_n = \left(\frac{-1}{4\pi^2} \right)^n \left(4^n - 1\right) \zeta(2n) && (11)
\end{aligned}$$

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

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

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

$$
\begin{aligned}
\widehat{\mathbf{y}} &= \frac{1}{2} - 2\sum_{m=1}^{\infty} b_m \left(2\boldsymbol{\theta}_2\left(\frac{1}{4} - \sum_{n=1}^{\infty} a_n(\boldsymbol{\theta}_1\mathbf{x})^{2n-1}\right)\right)^{2m-1} \qquad (13)\\
&= \frac{1}{2} - 2\sum_{m=1}^{\infty} 2^{2m-1} b_m \boldsymbol{\theta}_2^{2m-1}\left(\frac{1}{4} - a_1(\boldsymbol{\theta}_1\mathbf{x}) - a_2(\boldsymbol{\theta}_1\mathbf{x})^3 - \ldots\right)^{2m-1}\\
&= \frac{1}{2} - \sum_{m=1}^{\infty} 2^{2m} b_m \boldsymbol{\theta}_2^{2m-1}\left(v_0 + v_1 + \ldots\right)^{2m-1},\ v_0 = \frac{1}{4}, v_1 = -a_1\boldsymbol{\theta}_1\mathbf{x}, v_2 = \ldots\\
&= \frac{1}{2} - \sum_{m=1}^{\infty} 2^{2m} b_m \boldsymbol{\theta}_2^{2m-1} \sum_{k_1+k_2+\ldots+k_n=2m-1} \binom{2m-1}{k_0, k_1, k_2, \ldots, k_n} v_0^{k_0} v_1^{k_1} \ldots v_n^{k_n}\\
&= \frac{1}{2} - \sum_{m=1}^{\infty} \sum_{k_1+k_2+\ldots+k_n=2m-1} 2^{2m} b_m \boldsymbol{\theta}_2^{2m-1} \binom{2m-1}{k_0, k_1, k_2, \ldots, k_n} v_0^{k_0} v_1^{k_1} \ldots v_n^{k_n} \qquad (14)
\end{aligned}
$$

where

$$\binom{2m-1}{k_0, k_1, \ldots, k_n} = \frac{(2m-1)!}{k_0!k_1!\ldots k_n!}$$

How does dropout affect this?