PROJECTED NEURAL ADDITIVE MODELS AS UNIVERSAL APPROXIMATORS

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ABSTRACT

This article proves that any continuous multi-variable function can be approximated arbitrarily close by a linear combination of single-variable functions of the inputs in a projected space. Using a set of independent neural networks to parameterize these feature functions of the projected inputs, we introduce their linear combination as the projected neural additive model (PNAM): an extension of the neural additive model (NAM) (cf. Agarwal et al. (2021)) that now enables universal approximation. While the couplings of the input variables bestow the PNAM with the universal approximation property, they could diminish the interpretability intrinsic to the NAM. As such, we propose regularization and post hoc techniques to promote sparse solutions and enhance the interpretability of the PNAM. The single-variable characteristic of the bases also enables us to convert them into symbolic equations and dramatically reduces the number of required parameters. We provide results from numerical experiments on invariants in knot theory, and phase field theory for fracture of brittle solids to illustrate the expressivity and interpretability of the PNAM.[1]

1 INTRODUCTION

While deep neural networks have become popular for a multitude of tasks due to their expressivity, they come at the cost of interpretability (Murdoch et al., 2019). Of the myriad methods introduced to address this issue, Agarwal et al. (2021) propose an alternative architecture, coined the neural additive model (NAM), by altering the connectivity of the network such that it becomes a linear combination of single-variable functions of the input variables, parameterized by independent multi-layer perceptrons (MLPs). Although the values of these functions can provide a degree of interpretability, the linear nature of the NAM in turn limits its expressivity. As a result, Phan et al. (2025) propose the use of a learnable linear transformation before passing the inputs to the NAM (see Fig. 1), which we refer to as the projected neural additive model (PNAM), to enhance the expressivity of the model.

Contribution. In this work, we prove that the PNAM is a universal approximator, elucidating its ability to approximate any continuous function on a closed and bounded domain. In particular, we first prove the polynomial reproducing property of the PNAM for an arbitrary number of variables and orders, then employ the Stone–Weierstrass theorem to establish its universal approximation property. To rectify the reduction in interpretability that the linear transformation may induce, we introduce regularization techniques that (i) permit us to rank the importance of each input feature, (ii) penalize unnecessary couplings between the inputs, and (iii) promote sparse solutions. We also leverage the modularity of the PNAM to prune nonessential parameters before leveraging the single-variable characteristic of its bases to convert them into symbolic equations. We apply the resultant models for multi-output predictions. In the numerical experiments, we demonstrate the various utilities of the PNAM, enabling users to dictate their desired degrees of accuracy and sparsity.

[1] We will open-source our code after the double-blind review process.

Related work. The PNAM is one of many architecture-based models introduced to enhance the interpretability of deep neural networks without compromising their expressivity. Other neural network models include, but are not limited to, Kolmogorov–Arnold networks (KANs) (Liu et al., 2024), deep polynomial neural networks (Chrysos et al., 2022), and graph neural networks with inductive biases (Cranmer et al., 2020). In addition, related sparsification, pruning, and post hoc methods include the SINDy algorithm (Brunton et al., 2016), structural pruning (Fang et al., 2023), and gradient-based attribution (Sundararajan et al., 2017). We note that while the PNAM can lead to mathematical expressions, it is not ideal for recovering physical laws with precise functional forms due to the potentially large dimension of the linear transformation. We reserve such tasks for proven symbolic regression (SR) algorithms using reinforcement learning (Petersen et al., 2019), physics-inspired strategies (Udrescu & Tegmark, 2020), and genetic programming (Cranmer, 2023).

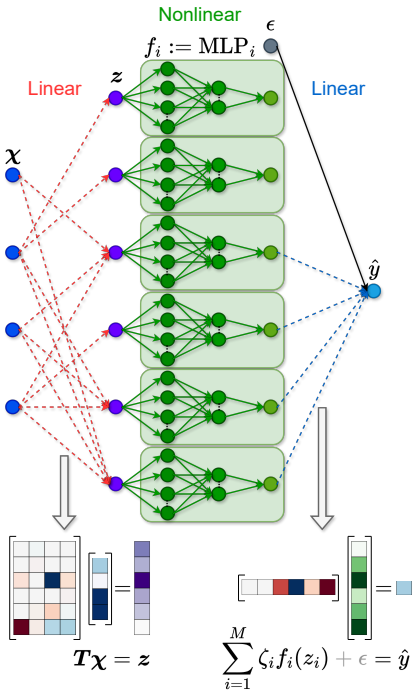

Figure 1: Architecture of the PNAM. The output $\widehat{y}$ is predicted via a linear combination of single-variable functions, parameterized by independent MLPs, which further are functions of linear combinations of the inputs $\boldsymbol{\chi}$. The transformation $\boldsymbol{T}$ and scaling coefficients $\boldsymbol{\zeta}$ (both denoted with dashed lines) can be optimized to yield sparser (and more interpretable) solutions.

2 Projected Neural Additive Models

2.1 Construction

Given a training data set $\{\boldsymbol{\mathcal{X}}, \boldsymbol{y}\} = \{(\boldsymbol{\chi}_j, y_j)\}_{j=1}^{D}$, where $\boldsymbol{\chi} = \{\chi_i\}_{i=1}^{N}$ is an input point, with N denoting the number of independent variables, y is the corresponding scalar output label, and D is the number of input-output pairs, the goal of supervised learning is to construct a function $\mathcal{F}$ that maps every input point to output label, that is, $y = \mathcal{F}(\boldsymbol{\chi})$: $\mathbb{R}^N \to \mathbb{R}$. Here, we hypothesize that the multi-variable function $\mathcal{F}$ can be approximated by a linear combination (or weighted sum) of single-variable functions $\{f_i\}_{i=1}^{M}$, with M denoting the number of feature functions, of the inputs in a projected space to produce the dependent variable:

$$\widehat{y} = \sum_{i=1}^{M} \zeta_i f_i \left(\sum_{j=1}^{N} T_{ij} \chi_j \right) + \epsilon = \sum_{i=1}^{M} g_i(z_i) + \epsilon, \quad (1)$$

where $\widehat{y}$ is a parameterization of y, and ϵ is an error term introduced to represent noise in the data. The projected variables $\boldsymbol{z}$ in Eq. 1 result from a linear transformation $\boldsymbol{T}$ of $\boldsymbol{\chi}$, that is, $\boldsymbol{z} = \boldsymbol{T}\boldsymbol{\chi}$: $\mathbb{R}^N \to \mathbb{R}^M$. Moreover, each single-variable function f_i: $\mathbb{R} \to \mathbb{R}$ and its corresponding scaling coefficient ζ_i are represented by the function g_i: $\mathbb{R} \to \mathbb{R}$ for compactness.

The feature functions $\{f_i\}$ in Eq. 1 can be constructed using polynomials or neural networks. Here, we parameterize y as a linear combination of MLPs:

$$\widehat{y} = \sum_{i=1}^{M} \zeta_i \text{MLP}_i \left(\sum_{j=1}^{N} T_{ij} \chi_j; \boldsymbol{W}_i^{(1)}, \ldots, \boldsymbol{W}_i^{(L)}, \boldsymbol{s}_i^{(1)}, \ldots, \boldsymbol{s}_i^{(L-1)} \right) + \epsilon, \quad (2)$$

where each f_i is an MLP with L layers, learnable weights $\left\{\boldsymbol{W}_i^{(1)}, \ldots, \boldsymbol{W}_i^{(L)}\right\}$ and biases $\left\{\boldsymbol{s}_i^{(1)}, \ldots, \boldsymbol{s}_i^{(L-1)}\right\}$, and element-wise activation function a:

$$\begin{aligned} &\text{MLP}_i \left(z_i; \boldsymbol{W}_i^{(1)}, \ldots, \boldsymbol{W}_i^{(L)}, \boldsymbol{s}_i^{(1)}, \ldots, \boldsymbol{s}_i^{(L-1)} \right) = \\ &\boldsymbol{W}_i^{(L)} a \left(\boldsymbol{W}_i^{(L-1)} a \left(\ldots a \left(\boldsymbol{W}_i^{(1)} z_i + \boldsymbol{s}_i^{(1)} \right) \ldots \right) + \boldsymbol{s}_i^{(L-1)} \right). \end{aligned} \quad (3)$$

To enable the model to learn high-frequency functions, a Fourier feature mapping (Tancik et al., 2020; Bahmani et al., 2024) can be leveraged to map a transformed input z_i to

$$\gamma_i(z_i) = [\cos(2\pi \boldsymbol{B}_i z_i)^{\mathrm{T}}, \sin(2\pi \boldsymbol{B}_i z_i)^{\mathrm{T}}]^{\mathrm{T}}, \tag{4}$$

where each entry in $\boldsymbol{B}_i$ is sampled from a Gaussian distribution $\mathcal{N}(0, \sigma^2)$ with standard deviation σ and is fixed after initialization, before passing it to Eq. 3. Let $\boldsymbol{\zeta} = \{\zeta_i\}_{i=1}^{M}$; as shown in Fig. 1, the transformation $\boldsymbol{T}$, scaling coefficients $\boldsymbol{\zeta}$, and error term ϵ in Eq. 2 can be encoded as two additional weight matrices and one bias term, respectively. A simpler version of this construction is first proposed in Phan et al. (2025) and corresponds to the PNAM, introduced (without a formal proof of universal approximation) to overcome the limited expressivity of the NAM (Agarwal et al., 2021).

2.2 Universal approximation

By the Stone–Weierstrass theorem (Stone, 1937; 1948; Cotter, 1990), polynomials are dense in the space of continuous functions, i.e., they can approximate any continuous function on a closed and bounded domain. As such, we can achieve universal approximation by reproducing polynomials. We show in Theorem A.1 that single-variable polynomials of the inputs in a projected space can be employed as the bases to approximate multi-variable polynomials. Instead of single-variable polynomials, one may also use the sum of one-dimensional (1D) neural networks of the projected inputs to achieve universal approximation. Since all such neural networks of single variables enjoy the universal approximation property (Hornik et al., 1989; Leshno et al., 1993; Lu et al., 2017), implying that they can approximate polynomials, we immediately get the universal approximation property of the resulting multi-dimensional neural network. This approximation capability is formally stated in the following theorem.

Theorem 2.1. *Let domain $\mathfrak{D}$ be a compact space of N dimensions, and let $\mathfrak{F}$ be a set of continuous real-valued functions on $\mathfrak{D}$, containing the identity function and satisfying separability and algebraic closure. For any $\epsilon > 0$ and any function $\mathcal{F}_1$ in $\mathcal{C}(\mathfrak{D})$, the set of continuous real-valued functions on $\mathfrak{D}$, there exists a polynomial $\mathcal{F}_2$ in $\mathfrak{F}$ such that*

$$|\mathcal{F}_1(\boldsymbol{\chi}) - \mathcal{F}_2(\boldsymbol{\chi})| < \epsilon, \tag{5}$$

for all $\boldsymbol{\chi} \in \mathfrak{D}$. Let $\mathfrak{G}$ be a set of single-variable polynomials or 1D neural networks. There exists a linear transformation $\boldsymbol{T}$: $\mathbb{R}^N \to \mathbb{R}^M$ and a set of functions $\{g_i$: $\mathbb{R} \to \mathbb{R}\}_{i=1}^{M}$ in $\mathfrak{G}$ such that

$$\mathcal{F}_2(\boldsymbol{\chi}) = \sum_{i=1}^{M} g_i \left(\sum_{j=1}^{N} T_{ij} \chi_j \right) \tag{6}$$

and, by extension,

$$\left| \mathcal{F}_1(\boldsymbol{\chi}) - \sum_{i=1}^{M} g_i \left(\sum_{j=1}^{N} T_{ij} \chi_j \right) \right| < \epsilon. \tag{7}$$

Proof. Equation 5 is the standard result of the Stone–Weierstrass theorem (Stone, 1937; 1948; Cotter, 1990), where $\mathcal{F}_2$ is a multi-variable polynomial. Furthermore, for the case where $\mathfrak{G}$ is a set of single-variable polynomials, Theorem A.1 proves that Eq. 6 is true. Thus, Eq. 7 follows. For the case where $\mathfrak{G}$ is a set of 1D fully connected feedforward neural networks (i.e., MLPs), its error bound may even be tighter than that of the former case for the same projection dimension M. Due to the universal approximation theorem of neural networks, single-variable MLPs that are sufficiently wide (Hornik et al., 1989) or deep (Lu et al., 2017) and use a non-polynomial activation function (Leshno et al., 1993) (e.g., the rectified linear unit (ReLU) function) can approximate not just polynomials, but any continuous function. □

2.3 Extension to multiple outputs

Now, let $\boldsymbol{y} = \{\{y_{ij}\}_{j=1}^{D}\}_{i=1}^{K}$, $\boldsymbol{\zeta} = \{\{\zeta_{ij}\}_{j=1}^{M}\}_{i=1}^{K}$, and $\boldsymbol{\epsilon} = \{\epsilon_i\}_{i=1}^{K}$, with K denoting the number of dependent variables. Equation 1 can be extended to multiple outputs $\{\widehat{y}_i\}$ as follows:

$$\widehat{y}_i = \sum_{j=1}^{M} \zeta_{ij} f_{ij} \left(\sum_{k=1}^{N} T_{jk} \chi_k \right) + \epsilon_i = \sum_{j=1}^{M} g_{ij}(z_j) + \epsilon_i, \qquad i = 1, 2, \ldots, K, \quad (\text{no sum over } i) \tag{8}$$

where f_{ij} is the i^{th} output of the j^{th} vector-valued function (Xu et al., 2023). To show that Eq. 8 is a natural extension of Eq. 1, consider the extreme case where the bases $\{g_{ij}\}$ share no common inputs $\{z_j\}$ across $\{\widehat{y}_i\}$. In that case, $M = \sum_{i=1}^{K} m_i$, with m_i denoting the number of dimensions required to approximate each $\widehat{y}_i$. Equivalently, for each index i, the number of indices j for which ζ_{ij} and f_{ij} are nonzero is m_i, yielding orthogonal bases $\{g_{ij}\}$. Along the lines of the universal approximation theorem associated with fully connected feedforward neural networks, M can be chosen to be arbitrarily large to approximate any set of continuous functions in theory.

2.4 Learning problem and constraints for sparsity

Let $\boldsymbol{\Theta} = \{\boldsymbol{\theta}_i\}_{i=1}^{M} = \left\{\left(\boldsymbol{W}_i^{(1)}, \ldots, \boldsymbol{W}_i^{(L)}, \boldsymbol{s}_i^{(1)}, \ldots, \boldsymbol{s}_i^{(L-1)}\right)\right\}_{i=1}^{M}$ denote all learnable parameters of the MLPs. We optimize the learnable parameters of the PNAM by minimizing the following loss function (in parentheses) for D training samples:

$$\begin{aligned}\boldsymbol{T}^*, \boldsymbol{\Theta}^*, \boldsymbol{\zeta}^*, \boldsymbol{\epsilon}^* = \underset{\boldsymbol{T}, \boldsymbol{\Theta}, \boldsymbol{\zeta}, \boldsymbol{\epsilon}}{\arg\min} \Bigg(& \mathcal{L}(\boldsymbol{y}, \widehat{\boldsymbol{y}}(\boldsymbol{\mathcal{X}}; \boldsymbol{T}, \boldsymbol{\Theta}, \boldsymbol{\zeta}, \boldsymbol{\epsilon})) + \mathcal{L}_{\text{P}} \\ & + \frac{1}{D}(w_1\ell_1 + w_2\ell_2) + \frac{1}{M}(w_3\ell_3 + w_4\ell_4 + w_5\ell_5)\Bigg),\end{aligned} \tag{9}$$

where

$$\mathcal{L} = -\frac{1}{D}\sum_{i=1}^{K}\sum_{j=1}^{D} y_{ij} \log \frac{\exp(\widehat{y}_i(\boldsymbol{\chi}_j; \boldsymbol{T}, \boldsymbol{\Theta}, \boldsymbol{\zeta}, \boldsymbol{\epsilon}))}{\sum_{k=1}^{K} \exp(\widehat{y}_k(\boldsymbol{\chi}_j; \boldsymbol{T}, \boldsymbol{\Theta}, \boldsymbol{\zeta}, \boldsymbol{\epsilon}))}$$

is the cross-entropy loss for classification, or

$$\mathcal{L} = \frac{1}{KD}\sum_{i=1}^{K}\sum_{j=1}^{D}(y_{ij} - \widehat{y}_i(\boldsymbol{\chi}_j; \boldsymbol{T}, \boldsymbol{\Theta}, \boldsymbol{\zeta}, \boldsymbol{\epsilon}))^2$$

is the mean squared error (MSE) for regression. Moreover, $\mathcal{L}_{\text{P}}$ can be employed to impose any additional physical constraints that restrict the space of admissible solutions (Czarnecki et al., 2017; Raissi et al., 2019; Bastek et al., 2024).

To prevent overfitting and produce interpretable solutions, we use the following two constraints:

$$\ell_1 = ||\boldsymbol{\Theta}||_2, \qquad \ell_2 = \left|\left|\{\{\{g_{ij}(\boldsymbol{\chi}_k; \boldsymbol{T}, \boldsymbol{\Theta}, \boldsymbol{\zeta})\}_{k=1}^{D}\}_{j=1}^{M}\}_{i=1}^{K}\right|\right|_2, \tag{10}$$

where ℓ_1 is the usual L_2 regularization of the weights and biases (Krogh & Hertz, 1991),[2] and ℓ_2 discourages $\{g_{ij}\}$ from taking on large values (Agarwal et al., 2021). Considering that the inputs and outputs are often scaled to small values in machine learning problems, the inclination for $\{g_{ij}\}$ to be small could be leveraged to determine the relative importance of the inputs. As we will exemplify later, if any element in the linear transformation $\boldsymbol{T}$ is relatively large, its corresponding input feature is more important than the others.

To further promote sparsity, we first define the singular value decomposition of $\boldsymbol{T}$ as follows:

$$\boldsymbol{T} = \boldsymbol{Q}_1 \boldsymbol{\Sigma} \boldsymbol{Q}_2^{\text{T}},$$

where $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$ are orthonormal matrices of dimensions $M \times M$ and $N \times N$, respectively, and $\boldsymbol{\Sigma}$ is an $M \times N$ diagonal matrix containing the $\min(M, N)$ singular values of $\boldsymbol{T}$. Based on the metric

$$\Phi(\boldsymbol{R}_1, \boldsymbol{R}_2) = ||\boldsymbol{I} - \boldsymbol{R}_1\boldsymbol{R}_2^{\text{T}}||_F = \sqrt{2(3 - \text{tr}(\boldsymbol{R}_1\boldsymbol{R}_2^{\text{T}}))}, \qquad \boldsymbol{R}_1, \boldsymbol{R}_2 \in SO(3),$$

described in Huynh (2009) for measuring the distance between two 3D rotations, we leverage

$$\ell_3 = \Phi(\boldsymbol{I}, \boldsymbol{Q}_1) + \Phi(\boldsymbol{I}, \boldsymbol{Q}_2) = \sqrt{2(M + N - (\text{tr}\boldsymbol{Q}_1 + \text{tr}\boldsymbol{Q}_2))} \tag{11}$$

to penalize unnecessary couplings between the inputs. In addition,

$$\ell_4 = ||\boldsymbol{T}||_1, \qquad \ell_5 = ||\boldsymbol{\zeta}||_1 \tag{12}$$

are employed to encourage nonessential coefficients in $\boldsymbol{T}$ and $\boldsymbol{\zeta}$ to go to zero (Tibshirani, 1996; Xu et al., 2023; Bahmani et al., 2024).

[2]We opt for $||\cdot||_2$ as opposed to $||\cdot||_2^2$ so that $\ell_1, \ell_2, \ldots, \ell_5$ are similar in magnitude, and thus, weighting coefficients $w_1, w_2, \ldots, w_5$ can be chosen within proximity of each other.

2.5 POST-PROCESSING AND SYMBOLIC REGRESSION

Upon successful training of the PNAM, post hoc analysis can be performed to further prune the model and enhance interpretability (Murdoch et al., 2019; Cheng et al., 2024). Due to the modularity of the PNAM, we propose three techniques to reduce the number of optimized parameters.

The first technique relies on the successful incorporation of the regularization term ℓ_2 in Eq. 10. Suppose the functions $\{g_{ij}\}$ are indeed small. In that case, we can examine the column-wise mean of the absolute values of the coefficients in the linear transformation (that is, $\frac{1}{M}\sum_{j=1}^{M}|T_{jk}|$), dubbed the mean absolute coefficients, to rank the importance of each input feature. Upon which, one may choose to keep only the top $n \leq N$ input features and zero out the columns of $\boldsymbol{T}$ associated with the $(N-n)$ less important features. The second technique entails selecting two hyperparameters T_0 and ζ_0 for which entries $T_{jk} < T_0$ and $\zeta_{ij} < \zeta_0$, for $k = 1, 2, \ldots, N$, $j = 1, 2, \ldots, M$, and $i = 1, 2, \ldots, K$, are set to zero.[3]

Finally, the third technique leverages the single-variable characteristic of the bases $\{g_{ij}\}$ to convert them into symbolic equations. Although any SR algorithm, such as DSR (Petersen et al., 2019) or AI Feynman (Udrescu & Tegmark, 2020), may be used to accomplish this task, here, we employ PySR (Cranmer, 2023), which utilizes genetic programming (Holland, 1992; Koza, 1994), for its extensive developer base and ease of use. To convert the i^{th} nonzero output of the j^{th} MLP into symbolic form, we employ the following loss function:

$$g_{ij}^{*} = \underset{g_{ij}}{\arg\min} \left(\frac{1}{D} \sum_{k=1}^{D} \left(\left(\zeta_{ij} \mathrm{MLP}_{ij}(z_j; \boldsymbol{\theta}_j)|_k - g_{ij}(z_j)|_k \right)^2 + w_6 \left(\zeta_{ij} \frac{\mathrm{d}\mathrm{MLP}_{ij}(z_j; \boldsymbol{\theta}_j)}{\mathrm{d}z_j}\bigg|_k - \frac{\mathrm{d}g_{ij}(z_j)}{\mathrm{d}z_j}\bigg|_k \right)^2 \right) \right), \quad (\text{no sum over } i \text{ and } j) \tag{13}$$

where $\{g_{ij}\}$ are mathematical expressions of single variables, and the weighting coefficient w_6 may be used to control the derivatives of the discovered functions. The sum of $\{g_{ij}\}$ over j (with $\{\epsilon_i\}$) then yields the outputs $\{\widehat{y}_i\}$ in Eq. 8. These post-processing steps can potentially reduce the tens of thousands of parameters of the PNAM to tens or hundreds of parameters, while alleviating the NP-hardness of multi-variable SR (Petersen et al., 2019; Virgolin & Pissis, 2022) and retaining the accuracy of deep neural networks.

3 NUMERICAL EXPERIMENTS

In the following experiments, we illustrate the expressivity and interpretability of the PNAM, afforded by the linear transformation and post hoc analysis. The first experiment leverages an extensive data set of mathematical knots from Davies et al. (2021) for (i) multi-label classification and (ii) single-task regression. The second experiment employs limited data from a phase field simulation of fracture propagation in Clayton et al. (2023) for multi-task regression, leveraging the additional physical constraint term $\mathcal{L}_{\mathrm{P}}$ in Eq. 9 and derivative information via the weighting coefficient w_6 in Eq. 13. If not specified, $\mathcal{L}_{\mathrm{P}}$ is not used and w_6 is set to zero in the experiment.

For all experiments, we hold out 20% of the data for testing; the remaining 80% undergo a training-validation split of 80 and 20%, respectively. The PNAM is implemented using the PyTorch deep learning library (Paszke et al., 2019) and SiLU[4] (Hendrycks & Gimpel, 2016; Elfwing et al., 2018) as the activation function a in Eq. 3. For the projection dimension M, we start with a square projection in every experiment and increase or decrease M as appropriate. Unless otherwise stated, we set weighting coefficients $w_1 = w_2 = w_3 = w_4 = w_5 = 0.01$ for all classification tasks and $w_1 = w_2 = w_3 = w_4 = w_5 = 0.001$ for all regression tasks. We use a batch size of 256 samples and the Adam optimizer (Kingma & Ba, 2014), employing an initial learning rate of 0.001 that decays by a factor of 0.995 after every epoch, to train all neural networks. Each model is trained 10 times

[3] Either the first, the second, or a combination of both techniques may be used. Like M, $w_1, w_2, \ldots, w_5$, and any other hyperparameters, the choices of n, T_0, and ζ_0 depend on the users and their desired degrees of accuracy and sparsity.

[4] We observe that ReLU results in a smaller loss $\mathcal{L}$ in Eq. 9 than SiLU, but the bases $\{g_{ij}\}$ that the PNAM learns are more chaotic/non-smooth and require more parameters/operations to approximate via Eq. 13.

Table 1: Performance of different neural network architectures for the multi-label classification problem of predicting the signature of mathematical knots. The first two rows are reproduced from Table 3 of Liu et al. (2024). See Liu et al. (2024) for definitions of G and k. In the next five rows, the mean and standard deviation of the test accuracy are computed from 10 runs. In the last row, the first hidden layer of the MLPs in the PNAM is replaced with a Fourier feature mapping (Eq. 4).

Method	Architecture	Parameter count	Test accuracy
DM's MLP	4 layers: [17, 300, 300, 300, 14]	3×10^5	78.0%
KAN	2 layers: [17, 1, 14] ($G = 3$, $k = 3$)	2×10^2	81.6%
Our MLP	3 layers: [17, 64, 32, 14]	1.2×10^4	$95.8 \pm 0.1\%$
NAM	3 layers: $17 \times [1, 64, 32, 14]$	2.1×10^5	$92.4 \pm 0.2\%$
PNAM	3 layers: $17 \times [1, 64, 32, 14]$	2.1×10^5	$95.0 \pm 0.2\%$
PNAM	3 layers: $8 \times [1, 64, 32, 14]$	9.8×10^4	$93.6 \pm 0.4\%$
PNAM	3 layers: $8 \times [1, 2(32), 32, 14]$ ($\sigma = 1$)	9.8×10^4	$94.3 \pm 0.3\%$

across 10 random seeds on a single NVIDIA A100-SXM4-40GB GPU. Each basis g_{ij} in Eq. 13 is evolved for one minute using 30 populations of 30 expressions with a maximum complexity of 30; all operators and leaf nodes have a complexity of one. Other relevant hyperparameters and training details are delineated with the results.

3.1 Benchmarking with knot theory

Established by a team of mostly Google DeepMind (DM) researchers (Davies et al., 2021), the data set of mathematical knots contains 243,746 samples, each possessing 17 geometric invariants: adjoint torsion degree, torsion degree, short geodesic (real part), short geodesic (imaginary part), injectivity radius, Chern–Simons invariant, cusp volume, longitudinal translation, meridional translation (imaginary part), meridional translation (real part), volume, and six symmetry groups. The goal of this problem is to use the aforementioned invariants to predict the signature of the knots, which can take on one of 14 values that are multiples of 2 from -12 to 14. As such, this task can be framed as a classification problem with 14 labels or a single-output regression problem; both options have been explored to benchmark performance.

Classification. The first two rows of Table 1 are reproduced from Liu et al. (2024), which compare the performance of the MLP[5] implemented by Davies et al. (2021) against that of the KAN. The next five rows detail our implementation of the MLP, the NAM, and three parameterizations of the PNAM, all using MLP(s) with two hidden layers of 64 and 32 neurons.[6] We scale all inputs to have zero mean and unit variance and train the models for 50 epochs without early stopping. All five models achieve test accuracy greater than 90%, with the MLP performing the best and the NAM performing the worst. Although the accuracy of the PNAM can be improved by increasing M (e.g., from 8 to 17) or replacing the first hidden layer of the MLPs with a Fourier feature mapping (e.g., with $\boldsymbol{B} \in \mathbb{R}^{32}$ and $\sigma = 1$), doing so increases the complexity of the learned functions.

For the PNAM with $M = 8$ and without the Fourier feature mapping, we present in Table 2 possible input variables that represent the three most important features by comparing the mean absolute coefficients of the linear transformation $\boldsymbol{T}$. Out of 10 runs, the meridional translation (real part) and longitudinal translation have the largest and second largest mean absolute coefficients, respectively, in all 10 runs, while the meridional translation (imaginary part) has the third largest mean absolute coefficient in seven runs. In addition, Table 2 reveals that keeping only coefficients in $\boldsymbol{T}$ associated with the top $n = 3$ inputs and zeroing out all other coefficients, the PNAM can still achieve a test accuracy of 78.1% (see Fig. A.1 for more information). Our findings are consistent with Fig. 3 of

[5]Inspections of the source code (`https://github.com/google-deepmind/mathematics_conjectures/blob/main/knot_theory.ipynb`) reveal that the training of the MLP is terminated when the validation loss increases (i.e., an early stopping patience of one evaluation is employed), which may have led to underfitting.

[6]The number of parameters of the MLP, NAM, and PNAM is estimated as $O(LW^2)$, $O(NLW^2)$, and $O(MLW^2)$, respectively, where W is the number of neurons in the widest layer.

Table 2: Ranking of important input features based on their mean absolute coefficients for the PNAM with $M = 8$ in the penultimate row of Table 1. The mean and standard deviation of the test accuracy associated with using only the top n features are computed from their frequency in 10 runs.

Rank	Input	Symbol	Frequency	Test accuracy
1	Re(meridional translation)	χ_{10}	10/10	$55.1 \pm 3.5\%$
2	Longitudinal translation	χ_8	10/10	$74.2 \pm 1.5\%$
3	Im(meridional translation)	χ_9	7/10	$78.1 \pm 2.4\%$
	Cusp volume	χ_7	1/10	80.5%
	Im(short geodesic)	χ_4	1/10	73.5%
	Volume	χ_{11}	1/10	70.5%

Davies et al. (2021)[7] and Fig. 4.3 of Liu et al. (2024), despite the fact that Davies et al. (2021) employ gradient-based attribution (Sundararajan et al., 2017) and Liu et al. (2024) leverage a specific KAN architecture with a hidden dimension of one to determine the relative importance of the inputs.

Regression. Davies et al. (2021) and Liu et al. (2024) then leverage the knowledge they acquire from the classification task to construct mathematical expressions for the signature of the knots, now as a single-output regression problem. Formula A in Table 3 corresponds to the equation handcrafted by Davies et al. (2021), and formulas B to F proceed from post-processing steps of KANs trained using only relevant invariants (Liu et al., 2024). Davies et al. (2021) originally report a test accuracy between 70–80% for formula A in their implementation, while Liu et al. (2024) report a test accuracy of 83.1%. Since the accuracy appears to be highly dependent on the test set that results from a random data split, we evaluate all formulas on our test set and the entire knot data set.

Here, we demonstrate that the PNAM in Table A.1—trained using all invariants and the same setup described in the classification task but without any knowledge of prior results—can be converted into symbolic equations with merely tens of parameters. We emphasize that formulas G to I in Table 3 are artificial constructs of the PNAM after pruning. Their particular forms are less crucial and would likely change as more analysis becomes available. Instead, what is crucial is the capability of the PNAM to discover pertinent relationships as new data and invariants are introduced.

Of the runs summarized in Table A.2, formulas H and I are obtained from the run depicted in Fig. A.2, with $n = 3$ and the cusp volume[8] as the third most important feature. Although the cusp volume is not explicitly stated in Davies et al. (2021) and Liu et al. (2024) as an invariant relevant for predictive accuracy, the PNAM discovers a potential relationship between the cusp volume and the signature of the knots that could improve accuracy. Furthermore, comparing formulas E and G suggests that the PNAM can achieve similar accuracy to the KAN despite the PNAM using only two invariants without relying on additional assumptions. For additional analyses of how the weighting coefficients in Eq. 9 affect the performance of the PNAM, see Fig. A.3.

3.2 Phase field theory for fracture of brittle solids

In this common solid mechanics problem, we explore the relationship between the expressivity of the PNAM and its projection dimension M. The data set simply contains 96 data points,[9] homogenized from a phase field simulation of fracture in boron carbide (B_4C) with isotropic elasticity and isotropic fracture energy from Clayton et al. (2023), for quasi-static extension up to peak load. Given the homogenized values of the axial strain, order parameter, and magnitude of the material gradient of the order parameter, the goal of this problem is to predict the average strain energy, phase energy, and axial stress. Considering that the stress is calculated as the derivative of the sum of the strain energy and phase energy with respect to the strain, we frame this task as a two-output regression problem. The MSE is employed as $\mathcal{L}$ in Eq. 9 to predict the strain energy and phase energy; to

[7] Note that Davies et al. (2021) swap the naming of the real and imaginary parts of the meridional translation in their code/figure (see footnote 5).

[8] The cusp volume is equivalent to the multiplication of the longitudinal translation and the imaginary part of the meridional translation (see Fig. 4.4(b) of Liu et al. (2024)).

[9] The phase field data set is open-source with our code and can be used to study the benign or catastrophic overfitting of overparameterized neural networks (Mallinar et al., 2022) for a physical system.

Table 3: Mathematical expressions for the knot data set. Inputs χ_7, χ_8, χ_9, and χ_{10} are the cusp volume, longitudinal translation, meridional translation (imaginary part), and meridional translation (real part), respectively. Formulas A to F are reproduced from Table 4 of Liu et al. (2024). A factor of $\frac{1}{2}$ is added to formula A for consistency with DeepMind's findings (Davies et al., 2021; 2024). Formula D has missing parentheses, so it cannot be evaluated. A factor of $\frac{1}{2}$ is added to formula E for consistency with formula A. For formulas G and H, bases $\{g_{ij}\}$ in Eq. 13 use addition, subtraction, multiplication, and square as operators; they additionally use exponential, sine, and tangent for formula I. Every constant is counted as a parameter. See our code to reproduce these results.

ID	Formula	PC†	Discovered by	Eval. of test acc.		Total acc.
				Reported	Our	
A	$\frac{\chi_8\chi_{10}}{2(\chi_{10}^2+\chi_9^2)}$	3	Human (DM)	83.1%	74.5%	73.8%
B	$-0.02\sin(4.98\chi_9+0.85)+0.08\lvert 4.02\chi_{10}+6.28\rvert-0.52-0.04e^{-0.88(1-0.45\chi_8)^2}$	12	[3, 1] KAN	62.6%	27.0%	26.8%
C	$0.17\tan(-1.51+0.1e^{-1.43(1-0.4\chi_9)^2+0.09e^{-0.06(1-0.21\chi_8)^2}}+1.32e^{-3.18(1-0.43\chi_{10})^2})$	17	[3, 1, 1] KAN	71.9%	41.7%	41.5%
D	$-0.09+1.04\exp(-9.59(-0.62\sin(0.61\chi_{10}+7.26))-0.32\tan(0.03\chi_8-6.59)+1-0.11e^{-1.77(0.31-\chi_9)^2)^2}-1.09e^{-7.6(0.65(1-0.01\chi_8)^3}+0.27\arctan(0.53\chi_9-0.6)+0.09+\exp(-2.58(1-0.36\chi_{10})^2))$	29	[3, 2, 1] KAN	84.0%	–	–
E	$\frac{4.76\chi_8\chi_{10}}{2(3.09\chi_9+6.05\chi_{10}^2+3.54\chi_9^2)}$	7	[3, 2, 1] KAN + Padé approx.	82.8%	79.3%	79.3%
F	$\frac{2.94-2.92(1-0.10\chi_{10})^2}{0.32(0.18-\chi_{10})^2+5.36(1-0.04\chi_8)^2+0.50}$	13	$\frac{[3,1]\text{ KAN}}{[3,1]\text{ KAN}}$	77.8%	27.0%	26.8%
G	$12.766(0.132(-\chi_{10}+0.035\chi_8+0.157)^2+0.592(-0.23\chi_{10}+0.008\chi_8+1)^2(0.162\chi_{10}-0.006\chi_8+0.076)-1)^4+7.202(0.871\chi_{10}+0.029\chi_8-(0.229\chi_{10}+0.008\chi_8-0.103)(0.229\chi_{10}+0.008\chi_8+0.159(\chi_{10}+0.033\chi_8-0.449)^2+0.625)-0.173)^2-10.643$	31	$8\times[1,64,32,1]$ PNAM ($n=2$)	–	75.9%	75.7%
H	$26((0.096\chi_{10}-0.002\chi_7+0.004\chi_8-0.237)(0.267\chi_{10}-0.004\chi_7+0.011\chi_8+0.119(\chi_{10}-0.016\chi_7+0.04\chi_8-0.316)^2-1)^2+0.133)(0.734\chi_{10}-0.012\chi_7+0.029\chi_8+0.418)+2.054(0.589\chi_{10}+0.018\chi_7-0.027\chi_8+1)^2-4.056(\chi_{10}+0.031\chi_7-0.046\chi_8+0.195)^2(0.107\chi_{10}+0.003\chi_7-0.005\chi_8-0.064(\chi_{10}+0.031\chi_7-0.046\chi_8+0.087(\chi_{10}+0.031\chi_7-0.046\chi_8-0.165(\chi_{10}+0.031\chi_7-0.046\chi_8+0.195)^2+0.195)^2+0.195)^2+1)^2-0.895$	52	$8\times[1,64,32,1]$ PNAM ($n=3$)	–	81.2%	80.9%
I	$2.574\chi_{10}+0.078\chi_7-0.13\chi_8+26(0.233(-\chi_{10}+0.016\chi_7-0.04\chi_8-0.597)^2\sin^2(0.367\chi_{10}-0.006\chi_7+0.015\chi_8-0.719)+\sin(0.777\chi_{10}-0.013\chi_7+0.031\chi_8+0.262))(0.168\chi_{10}-0.003\chi_7+0.007\chi_8-0.053)+15.626(-\sin(0.54\chi_{10}+0.017\chi_7-0.025\chi_8+0.105)-0.049)^2(-0.165\chi_{10}-0.005\chi_7+0.008\chi_8-0.645)+0.509$	34	$8\times[1,64,32,1]$ PNAM ($n=3$)	–	81.4%	81.0%

† Parameter count is abbreviated as PC.

predict the stress, we use the following form of the constraint term $\mathcal{L}_{\mathrm{P}}$:[10]

$$\mathcal{L}_{\mathrm{P}}=\frac{w_{\mathrm{P1}}}{D}\sum_{k=1}^{D}\left((y'_{1,1}+y'_{2,1})|_k-\left.\frac{\partial(\widehat{y}_1(\boldsymbol{\chi};\boldsymbol{T},\boldsymbol{\Theta},\boldsymbol{\zeta},\boldsymbol{\epsilon})+\widehat{y}_2(\boldsymbol{\chi};\boldsymbol{T},\boldsymbol{\Theta},\boldsymbol{\zeta},\boldsymbol{\epsilon}))}{\partial\chi_1}\right|_k\right)^2,$$

where $y'_{1,1}$ and $y'_{2,1}$ are the derivatives of the strain energy and phase energy, respectively, with respect to the strain (χ_1). We set the weighting coefficient $w_{\mathrm{P1}}=1$.

All variables are scaled to have zero min and unit max. Table 4 depicts the performance of the MLP, the NAM, and four parameterizations of the PNAM, all using MLP(s) with three hidden layers of 256 neurons and set to train for 5000 epochs with an early stopping patience of 50 epochs. On average, the test MSE of the PNAM decreases as we increase M (cf. Phan et al. (2025)). Nevertheless, a run of the PNAM with $M=8$ turns out to be the model that achieves the smallest MSE. Therefore, we leverage $w_6=1$ in Eq. 13, which ensures accurate predictions of the stress, to convert this neural

[10] Ginzburg–Landau kinetics (Gurtin, 1996), or its quasi-static reduction in the present case, could be added as a constraint if one has access to the loading rate and the Laplacian of the order parameter. See Miehe et al. (2010) for background on phase field fracture mechanics and corresponding numerical models.

Table 4: Performance of different neural network architectures for the multi-output regression problem of predicting the strain energy, phase energy, and stress. The mean and standard deviation of the test MSE for all three variables are computed from 10 runs.

Method	Architecture	Parameter count	Test MSE
MLP	4 layers: [3, 256, 256, 256, 2]	2.6×10^5	$(7.05 \pm 2.02) \times 10^{-5}$
NAM	4 layers: $3 \times [1, 256, 256, 256, 2]$	7.9×10^5	$(1.12 \pm 0.62) \times 10^{-4}$
PNAM	4 layers: $3 \times [1, 256, 256, 256, 2]$	7.9×10^5	$(3.31 \pm 2.11) \times 10^{-4}$
PNAM	4 layers: $8 \times [1, 256, 256, 256, 2]$	2.1×10^6	$(1.34 \pm 0.91) \times 10^{-4}$
PNAM	4 layers: $16 \times [1, 256, 256, 256, 2]$	4.2×10^6	$(8.01 \pm 3.76) \times 10^{-5}$
PNAM	4 layers: $32 \times [1, 256, 256, 256, 2]$	8.4×10^6	$(6.47 \pm 2.71) \times 10^{-5}$

Table 5: Mathematical expressions for the phase field data set. Inputs χ_1, χ_2, and χ_3 are the strain, order parameter, and material gradient of the order parameter, respectively. To convert the PNAM with $M = 8$ in Table 4 and $T_0 = \zeta_0 = 0.05$ into symbolic form, bases $\{g_{ij}\}$ in Eq. 13 use addition, subtraction, multiplication, and square as operators. Counting every constant in $\{g_{ij}\}$ and $\{z_j\}$ as a parameter, the symbolic form has 112 parameters and achieves a test MSE of 2.25×10^{-5}.

Basis	Formula	Input	Formula
$g_{1,1}$	$-z_1^3 + 1.524z_1^2 + z_1 + ((-z_1 + (z_1 - 0.028)^2 + 0.75)^2 - 0.102)^2 - 0.269$	z_1	$203.741\chi_1 + 1.87\chi_2 - 3.048\chi_3$
$g_{2,1}$	$z_1^2 - (z_1 - 0.597)(z_1 - 0.291)(1.378z_1(0.786z_1 - 1)^4 + 0.525z_1 - 0.074) - 0.093$		
$g_{1,2}$	$z_2^3(0.147 - 0.074z_2) + 0.383z_2^2 + 0.119z_2 - 0.119$	z_2	$235.816\chi_1 - 0.461\chi_2 + 2.333\chi_3$
$g_{2,2}$	$-10.229z_2(0.003 - 0.002z_2^2) + 0.011$		
$g_{1,3}$	$0.967z_3(z_3 - 1.108)(-3.255z_3^3 + z_3 - 1.418) - 2z_3 + 0.07$	z_3	$-114.828\chi_1 + 1.284\chi_2 + 12.089\chi_3$
$g_{2,3}$	$1.046z_3 + 2.265(z_3 - 0.403)^2(0.65z_3^3 - z_3^2 + 0.835)^2 - 0.25$		
$g_{1,4}$	$-z_4(0.009z_4 + 0.069) + 0.005$	z_4	$-185.754\chi_1 + 1.866\chi_2 + 2.19\chi_3$
$g_{2,4}$	0		
$g_{1,5}$	$0.118z_5(2z_5 + 0.217)(0.033z_5^2(z_5 + 1) - z_5 + 3.239) - 0.116$	z_5	$190.698\chi_1 + 0.282\chi_2 + 6.271\chi_3$
$g_{2,5}$	$-z_5(-0.03z_5 + 0.003(0.772z_5(z_5 - 0.466)^2 - z_5 + 0.596)^2 + 0.009) - 0.002$		
$g_{1,6}$	0	z_6	$1.503\chi_2$
$g_{2,6}$	$z_6(0.003z_6^2 + 0.009z_6 - 0.043) + 0.016$		
$g_{1,7}$	$z_7(z_7^2(z_7^{10}(z_7 + 0.917)^2 - 0.014) + 0.079z_7 - 0.087) - 0.029$	z_7	$-119.681\chi_1 + 0.531\chi_2 - 5.929\chi_3$
$g_{2,7}$	$-0.004z_7^3 + 0.009z_7^2 + 0.024z_7 + 0.007$		
$g_{1,8}$	$0.003 - 0.009z_8$	z_8	$-27.984\chi_1 - 0.769\chi_2 + 6.628\chi_3$
$g_{2,8}$	0		

network model with approximately 10^6 parameters into symbolic form with roughly 100 parameters. As illustrated in Figs. A.4 and A.5, by employing SiLU as the activation function a in Eq. 3, we are able to approximate all bases $\{g_{ij}\}$ as polynomials of single variables in Table 5. Predictions of the strain energy, phase energy, and stress for the linear combinations of these polynomials are portrayed in Fig. A.6, achieving a test MSE of 2.25×10^{-5}.

4 Conclusion

We prove the universal approximation property of the PNAM and demonstrate its superior prediction capability compared to the NAM in two numerical experiments. By increasing the dimension of the linear transformation, the PNAM can achieve similar performance to or even outperform the MLP. Moreover, we leverage the modularity of the PNAM to gain insight into important input features, prune unnecessary parameters, and convert the model into symbolic form. However, as a stand-alone model, the PNAM is not meant to replace the MLP, NAM, or even classical SR. Rather, it serves as an alternative to obtain a better trade-off between expressivity and interpretability—achieving the accuracy of the MLP and retaining a degree of interpretability of the NAM, all while being relatively straightforward to train. Further studies are required before we can recommend the PNAM, because of its modularity, as a backbone in graph neural networks or transformers, which may enable us to prune the vast number of parameters of these models and accelerate inference during test time.

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A Appendix

A.1 Polynomial reproducing

Here, we prove the polynomial reproducing property, namely, any multi-variable polynomial $\mathcal{F}$ of $\boldsymbol{\chi} \in \mathbb{R}^N$ can be reproduced by a linear combination of $\{g_i\}$, where $g_i(z_i)$ is a single-variable polynomial of $z_i = \sum_{j=1}^{N} T_{ij}\chi_j$, for each $i = 1, 2, \ldots, M$. The main proof can be established for arbitrary dimensions with mathematical induction. The base case for this proof by induction is conducted in two dimensions.

First, we present a lemma that verifies the reproducing property for a special case in two dimensions, which can be used to prove the general case.

Lemma A.1. *For any monomial $\chi_1^p\chi_2^q$, there exists a linear transformation $\boldsymbol{T}$: $\mathbb{R}^N \to \mathbb{R}^M$, where $N = 2$ and $M = p + q + 1$, with $T_{i1} = 1$ and $T_{i2} = c_i$, and a set of coefficients $\{\zeta_i\}$ such that*

$$\chi_1^p\chi_2^q = \sum_{i=1}^{M} \zeta_i \left(\sum_{j=1}^{N} T_{ij}\chi_j \right)^{M-1} = \sum_{i=1}^{M} \zeta_i (\chi_1 + c_i\chi_2)^{p+q}. \tag{A.1}$$

Proof. Let us expand each term of the summation on the right-hand side of Eq. A.1 and collect terms with the same polynomial orders. We get the following equivalent form:

$$\begin{aligned} \chi_1^p\chi_2^q &= \sum_{i=1}^{M} \zeta_i (\chi_1 + c_i\chi_2)^{p+q} \\ &= \sum_{m=0}^{p+q} \sum_{i=1}^{M} c_i^{p+q-m} \zeta_i \begin{pmatrix} p+q \\ m \end{pmatrix} \chi_1^m \chi_2^{p+q-m}. \end{aligned}$$

Comparing the coefficients of the polynomials on both sides, for any choice of $\{c_i\}$, we end up with an $M \times M$ system of linear equations for $\{\zeta_i\}$ as follows:

$$\begin{bmatrix} c_1^{p+q} & c_2^{p+q} & c_3^{p+q} & \ldots & c_M^{p+q} \\ c_1^{p+q-1} & c_2^{p+q-1} & c_3^{p+q-1} & \ldots & c_M^{p+q-1} \\ c_1^{p+q-2} & c_2^{p+q-2} & c_3^{p+q-2} & \ldots & c_M^{p+q-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \ldots & 1 \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \vdots \\ \zeta_M \end{bmatrix} = \delta_{mp} \begin{bmatrix} 1 \\ \frac{1}{p+q} \\ \begin{pmatrix} p+q \\ 2 \end{pmatrix}^{-1} \\ \vdots \\ 1 \end{bmatrix},$$

where δ_{mp} is the Kronecker delta. Each equation of the linear system can be written compactly as

$$\sum_{i=1}^{M} c_i^{p+q-m}\zeta_i = \delta_{mp}\begin{pmatrix} p+q \\ m \end{pmatrix}^{-1}, \qquad m = 0, 1, \ldots, p+q.$$

To show that we can find $\{c_i, \zeta_i\}$ satisfying the system, we note that the coefficient matrix forms a so-called Vandermonde matrix (Macon & Spitzbart, 1958; Turner, 1966), which is invertible as long as $\{c_i\}$ is taken to be any set of mutually different constants, that is, $c_i \neq c_j$ for $i \neq j$. This completes the proof. □

Even for this simple case, we may observe the nonuniqueness in the construction of the linear transformation. Therefore, it is reasonable to expect that, for specific application problems involving machine learning, one may optimize the transformation to achieve effective representations in a possibly low-dimensional feature space. We give some illustrations in the following example.

Example A.1. *We present some instances where the actual value of M could be smaller than $p + q + 1$. In fact, for $p = q = 1$, we have*

$$\chi_1\chi_2 = \left(\chi_1 + \frac{1}{4}\chi_2\right)^2 - \left(\chi_1 - \frac{1}{4}\chi_2\right)^2,$$

corresponding to $M = 2$. For the trivial case of $p = 0$ or $q = 0$, we may simply use the identity transformation with $M = N = 1$. There are also examples that have a smaller value of M than the input dimension $N = 2$, such as $\chi_1^2 + 2\chi_1\chi_2 + \chi_2^2 = z_1^2$, where $z_1 = \chi_1 + \chi_2$, for which $M = 1 < 2 = N$. This again illustrates the effect of possible dimensionality reduction via a suitable transformation.

Next, we consider the extension of Lemma A.1. Since a product of polynomials of single variables $f_1(\chi_1)$ and $f_2(\chi_2)$ can be written as linear combinations of monomials $\{\chi_1^p\chi_2^q\}$, Lemma A.1 can easily be extended to a slightly more general form.

Lemma A.2. *For any polynomial of $(\chi_1, \chi_2) \in \mathbb{R}^2$ having the product form $f_1(\chi_1)f_2(\chi_2)$, there exists a linear transformation $\boldsymbol{T}$: $\mathbb{R}^2 \to \mathbb{R}^M$, where $M = \deg(f_1) + \deg(f_2) + 1$, and a set of single-variable polynomials $\{g_i\colon \mathbb{R} \to \mathbb{R}\}_{i=1}^M$ such that*

$$f_1(\chi_1)f_2(\chi_2) = \sum_{i=1}^{M} g_i(T_{i1}\chi_1 + T_{i2}\chi_2). \tag{A.2}$$

Proof. Let us express the two single-variable polynomials as

$$f_1(\chi_1) = \sum_p a_p\chi_1^p, \qquad f_2(\chi_2) = \sum_q b_q\chi_2^q.$$

Expanding the product on the left-hand side of Eq. A.2 and applying Lemma A.1 to each term in the product, we get

$$f_1(\chi_1)f_2(\chi_2) = \sum_{p=0}^{\deg(f_1)}\sum_{q=0}^{\deg(f_2)} a_p b_q \sum_{i=1}^{p+q+1} \zeta_{pqi}(\chi_1 + c_{pqi}\chi_2)^{p+q},$$

where subscripts p and q are introduced for $\{c_i, \zeta_i\}$ to elucidate that a different transformation $\boldsymbol{T}$ of dimensions $(p+q+1)\times 2$ is employed for each monomial. However, due to the freedom of choice in the construction of each $\boldsymbol{T}$, the same $\boldsymbol{T}$ of dimensions $(\deg(f_1) + \deg(f_2) + 1)\times 2$ can be used for all pairwise product terms. This choice stems from the fact that the innermost summation has a final upper limit of $M = \deg(f_1) + \deg(f_2) + 1$. Replacing $p + q + 1$ and c_{pqi} with M and c_i, respectively, we can move this summation to the outside:

$$f_1(\chi_1)f_2(\chi_2) = \sum_{i=1}^{M}\sum_{p=0}^{\deg(f_1)}\sum_{q=0}^{\deg(f_2)} a_p b_q \zeta_{pqi}(\chi_1 + c_i\chi_2)^{p+q},$$

resulting in Eq. A.2, where

$$g_i(T_{i1}\chi_1 + T_{i2}\chi_2) = \sum_p\sum_q a_p b_q \zeta_{pqi}(\chi_1 + c_i\chi_2)^{p+q}; \qquad T_{i1} = 1, \qquad T_{i2} = c_i.$$

□

Another consequence is the reproducing property for arbitrary polynomials in two dimensions.

Lemma A.3. *For any polynomial $\mathcal{F} = \mathcal{F}(\chi_1, \chi_2)$ of $(\chi_1, \chi_2) \in \mathbb{R}^2$, there exists a linear transformation $\boldsymbol{T}$: $\mathbb{R}^2 \to \mathbb{R}^M$, where $M = \deg(\mathcal{F}) + 1$, and a set of single-variable polynomials $\{g_i$: $\mathbb{R} \to \mathbb{R}\}_{i=1}^M$ such that*

$$\mathcal{F}(\chi_1, \chi_2) = \sum_{i=1}^{M} g_i(T_{i1}\chi_1 + T_{i2}\chi_2). \tag{A.3}$$

Proof. Note that $\deg(\mathcal{F})$ refers to the degree of the multi-variable polynomial, given by the highest degree of the monomials $\{\chi_1^p \chi_2^q\}$ in $\mathcal{F}$. Lemma A.3 can be proved by expanding $\mathcal{F}(\chi_1, \chi_2)$, which produces the same set of monomials as the product of $f_1(\chi_1)$ and $f_2(\chi_2)$ in Lemma A.2, where $\deg(\mathcal{F}) = \deg(f_1) + \deg(f_2)$. This realization concludes the proof. □

Finally, we employ mathematical induction to extend the result to any input dimension.

Theorem A.1. *For any polynomial $\mathcal{F} = \mathcal{F}(\boldsymbol{\chi}) = \mathcal{F}(\chi_1, \ldots, \chi_N)$ of $\boldsymbol{\chi} \in \mathbb{R}^N$, there exists a linear transformation $\boldsymbol{T}$: $\mathbb{R}^N \to \mathbb{R}^M$, for some M that could be chosen to depend only on $\deg(\mathcal{F})$ and N (e.g., $M = \deg(\mathcal{F}) + N - 1$), and a set of single-variable polynomials $\{g_i$: $\mathbb{R} \to \mathbb{R}\}_{i=1}^M$ such that*

$$\mathcal{F}(\chi_1, \ldots, \chi_N) = \sum_{i=1}^{M} g_i \left(\sum_{j=1}^{N} T_{ij}\chi_j \right). \tag{A.4}$$

Proof. Once we have shown that Theorem A.1 holds for a particular input dimension (e.g., $N = 2$), by leveraging the inductive hypothesis to show that it also holds for $N + 1$, the theorem must hold for all subsequent N, in accordance with the principle of mathematical induction. For $N = 2$, the polynomial reproducing property has been proved in Lemma A.3.

Assume that Theorem A.1 holds for an arbitrary input dimension N. We then consider a polynomial $\mathcal{F} = \mathcal{F}(\chi_1, \ldots, \chi_N, \chi_{N+1})$. It can be written as

$$\mathcal{F}(\chi_1, \ldots, \chi_N, \chi_{N+1}) = \sum_{p=0}^{P} \mathcal{F}_p(\chi_1, \ldots, \chi_N)\chi_{N+1}^p,$$

for some polynomials $\{\mathcal{F}_p\}_{p=0}^P$. By the inductive hypothesis, we have a linear transformation $\boldsymbol{T}_{\mathfrak{N}}$: $\mathbb{R}^N \to \mathbb{R}^{M_{\mathfrak{N}}}$ and a set of polynomials $\{\{\widetilde{g}_{pi}\}_{i=1}^{M_{\mathfrak{N}}}\}_{p=0}^P$ such that

$$\mathcal{F}_p(\chi_1, \ldots, \chi_N) = \sum_{i=1}^{M_{\mathfrak{N}}} \widetilde{g}_{pi}(z_{\mathfrak{N},i}), \qquad z_{\mathfrak{N},i} = \sum_{j=1}^{N} T_{\mathfrak{N},ij}\chi_j. \tag{A.5}$$

As a result,

$$\mathcal{F}(\chi_1, \ldots, \chi_N, \chi_{N+1}) = \sum_{p=0}^{P} \sum_{i=1}^{M_{\mathfrak{N}}} \widetilde{g}_{pi}(z_{\mathfrak{N},i})\chi_{N+1}^p.$$

By Lemma A.2, for each product term $\widetilde{g}_{pi}(z_{\mathfrak{N},i})\chi_{N+1}^p$ in the summation, there exists a linear transformation $\widetilde{\boldsymbol{T}}_{\mathfrak{N}}$ that maps any pair $(z_{\mathfrak{N},i}, \chi_{N+1})$ to $\mathbb{R}^{M_{\mathfrak{N}+1}}$ such that, for each choice of the indices p and i, the product $\widetilde{g}_{pi}(z_{\mathfrak{N},i})\chi_{N+1}^p$ is a sum of single-variable polynomials in the transformed space $\mathbb{R}^{M_{\mathfrak{N}+1}}$, where

$$M_{\mathfrak{N}} + P = M_{\mathfrak{N}+1} = \deg(\mathcal{F}) + N.$$

Composing $\boldsymbol{T}_{\mathfrak{N}}$ together with all $\widetilde{\boldsymbol{T}}_{\mathfrak{N}}$, we get a linear transformation $\boldsymbol{T}_{\mathfrak{N}+1}$ from $\mathbb{R}^{N+1}$ to $\mathbb{R}^{M_{\mathfrak{N}+1}}$ such that $\mathcal{F}(\chi_1, \ldots, \chi_N, \chi_{N+1})$ is a linear combination of polynomials $\{g_i\}_{i=1}^{M_{\mathfrak{N}+1}}$ of single variables $\boldsymbol{z} \in \mathbb{R}^{M_{\mathfrak{N}+1}}$. Thus, Theorem A.1 holds for input dimension $N + 1$. This completes the induction process and the proof. □

As noted in Example A.1, due to the nonuniqueness of the transformation, it is possible to achieve more effective and potentially low-dimensional representations through learning and optimization.

A.2 Additional results for knot theory: classification

Figure A.1 shows a complete ranking of the inputs and the associated test accuracy of using the top n inputs from one of the runs summarized in Table 2.

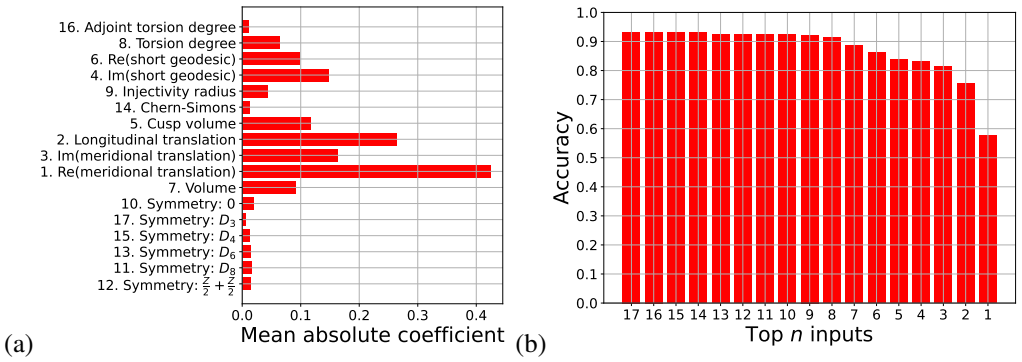


Figure A.1: One complete instance of the ranking and accuracy reported in Table 2. (a) Relative importance of the input features based on their mean absolute coefficients, and (b) test accuracy associated with using the top n features in (a).

A.3 Additional results for knot theory: regression

Table A.1 compares the performance of the NAM with 17 bases against that of the PNAM with eight bases, both of which can be converted into symbolic equations after training. Considering the poor performance of the NAM, we proceed with just the PNAM. Similar to Table 2, Table A.2 suggests that the meridional translation (real part) and longitudinal translation are the most and second most important invariants, respectively. Nevertheless, solely comparing the mean absolute coefficients is not ideal, as unimportant features can be ranked as important. We can, however, eliminate these features by examining the accuracy associated with including them, since including an unimportant feature does not improve the accuracy compared to the corresponding case with one less input.

Table A.1: Performance of the NAM and PNAM for the single-output regression problem of predicting the signature of mathematical knots. The mean and standard deviation of the test accuracy are computed from 10 runs.

Method	Architecture	Parameter count	Test accuracy
NAM	3 layers: $17 \times [1, 64, 32, 1]$	2.1×10^5	$65.0 \pm 0.2\%$
PNAM	3 layers: $8 \times [1, 64, 32, 1]$	9.8×10^4	$85.5 \pm 0.3\%$

Table A.2: Ranking of important input features based on their mean absolute coefficients for the PNAM in Table A.1. The mean and standard deviation of the test accuracy associated with using only the top n features are computed from their frequency in 10 runs.

Rank	Input	Symbol	Frequency	Test accuracy
1	Re(meridional translation)	χ_{10}	10/10	$55.7 \pm 1.2\%$
2	Longitudinal translation	χ_8	6/10	$74.8 \pm 1.4\%$
	Torsion degree	χ_2	4/10	$54.9 \pm 0.5\%$
3	Torsion degree	χ_2	3/10	$76.4 \pm 0.4\%$
	Re(short geodesic)	χ_3	3/10	$61.8 \pm 7.3\%$
	Longitudinal translation	χ_8	2/10	$76.5 \pm 0.2\%$
	Cusp volume	χ_7	1/10	81.3%
	Im(short geodesic)	χ_4	1/10	74.3%

Figure A.2 shows a complete ranking of the inputs and the associated test accuracy of using the top n inputs from one of the runs summarized in Table A.2. The ranking in Fig. A.2(d) is determined from the mean absolute coefficients of the linear transformation $\boldsymbol{T}$ in Fig. A.2(b). This linear transformation (i) consists mainly of diagonal elements due to the constraint ℓ_3 in Eq. 11 and (ii) is sparse due to the constraint ℓ_4 in Eq. 12. The transformation $\boldsymbol{T}$ with $n = 3$ in Fig. A.2(c) and the scaling coefficients $\boldsymbol{\zeta}$ of just two nonzero bases in Fig. A.1(a) are leveraged to construct formulas H and I in Table 3, which have comparable test accuracy to Fig. A.1(e) for $n = 3$.

Recall that these results correspond to weighting coefficients $w_1 = w_2 = w_3 = w_4 = w_5 = 0.001$, chosen to balance the trade-off between accuracy and sparsity. Figure A.3(b) reveals that setting $w_1 = w_2 = w_3 = w_4 = w_5 = 0$ improves (reduces) the accuracy for large (small) n due to the extensive number of coefficients with large values (the erroneous ranking of the input features) in Fig. A.3(a). Although the exact ranking may not be correct, the PNAM can still narrow down a set of variables (e.g., $n = 6$) that contains some of the most important variables. On the other hand, setting $w_1 = w_2 = w_3 = w_4 = w_5 = 0.01$ results in such a sparse $\boldsymbol{T}$ (see the small coefficient values in Fig. A.3(c)) such that the accuracy in Fig. A.3(d) is poor regardless of n.

A.4 Additional results for phase field theory

The polynomials $\{g_{ij}\}$ in Table 5, along with their derivatives, are plotted and compared with their neural network parameterizations in Figs. A.4 and A.5. We provide test predictions of the average strain energy, phase energy, and axial stress for the linear combinations of these polynomials in Fig. A.6.

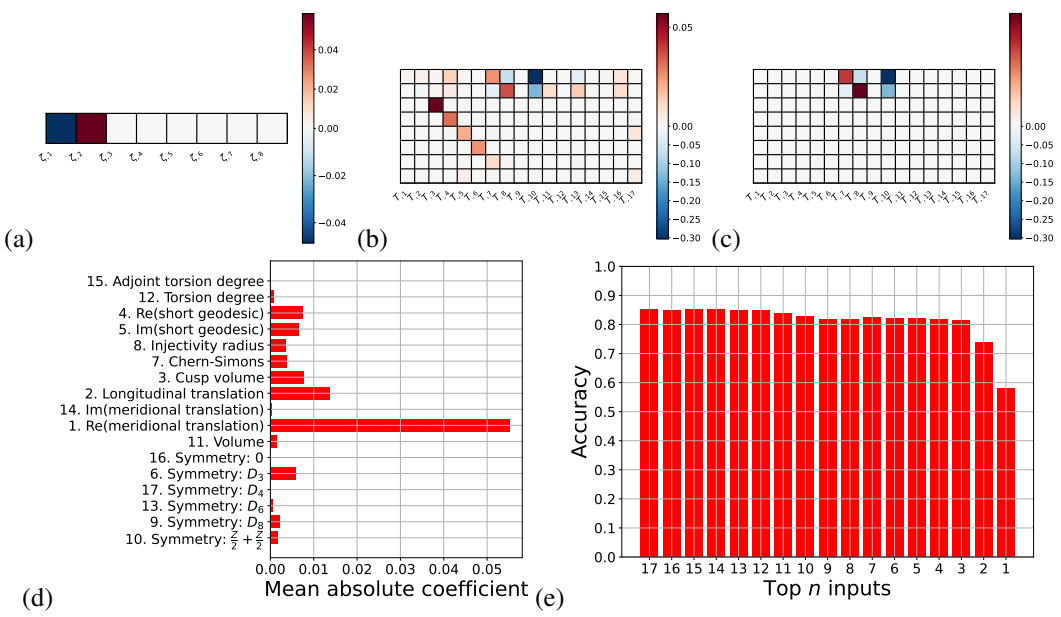


Figure A.2: One complete instance of the ranking and accuracy reported in Table A.2, along with the optimized parameters. (a) Unmodified scaling coefficients $\boldsymbol{\zeta}$, (b) unmodified linear transformation $\boldsymbol{T}$, (c) $\boldsymbol{T}$ with $n = 3$ and rows corresponding to columns of $\boldsymbol{\zeta}$ in (a) having a value of zero eliminated, (d) relative importance of the input features based on their mean absolute coefficients of $\boldsymbol{T}$ in (b), and (e) test accuracy associated with using the top n features in (d).

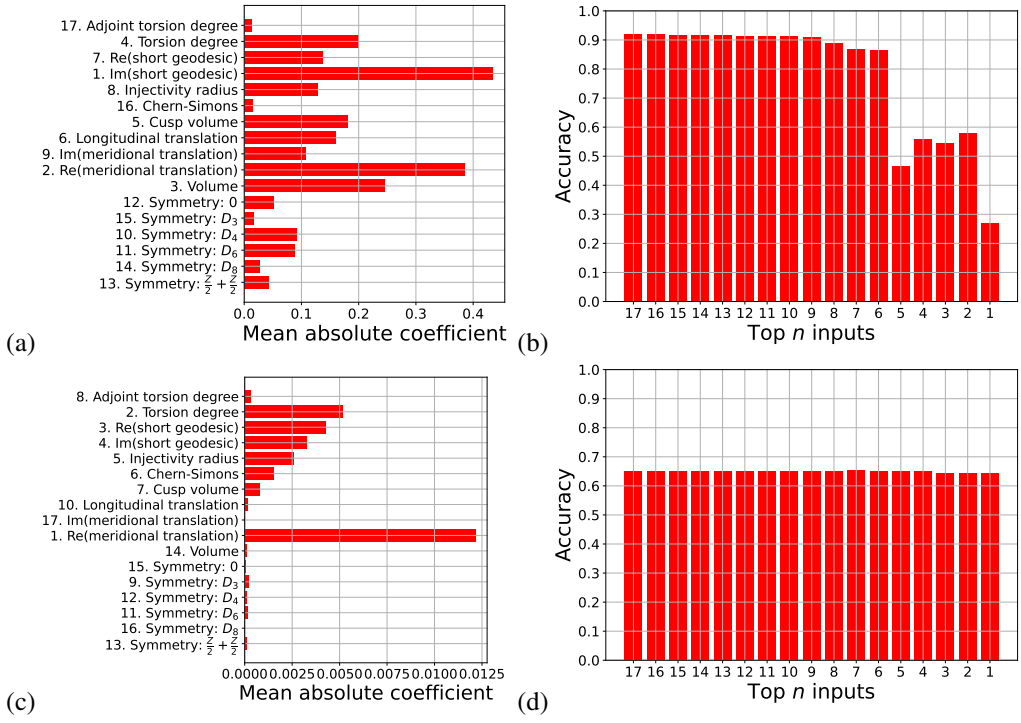


Figure A.3: Effects of weighting coefficients $w_1, w_2, \ldots, w_5$ for a PNAM with the same architecture as the PNAM in Table A.1. Weighting coefficients $w_1 = w_2 = w_3 = w_4 = w_5 = 0$ for (a) and (b); $w_1 = w_2 = w_3 = w_4 = w_5 = 0.01$ for (c) and (d). (a) and (c): Relative importance of the input features based on their mean absolute coefficients. (b) and (d): Test accuracy associated with using the top n features in (a) and (c), respectively.

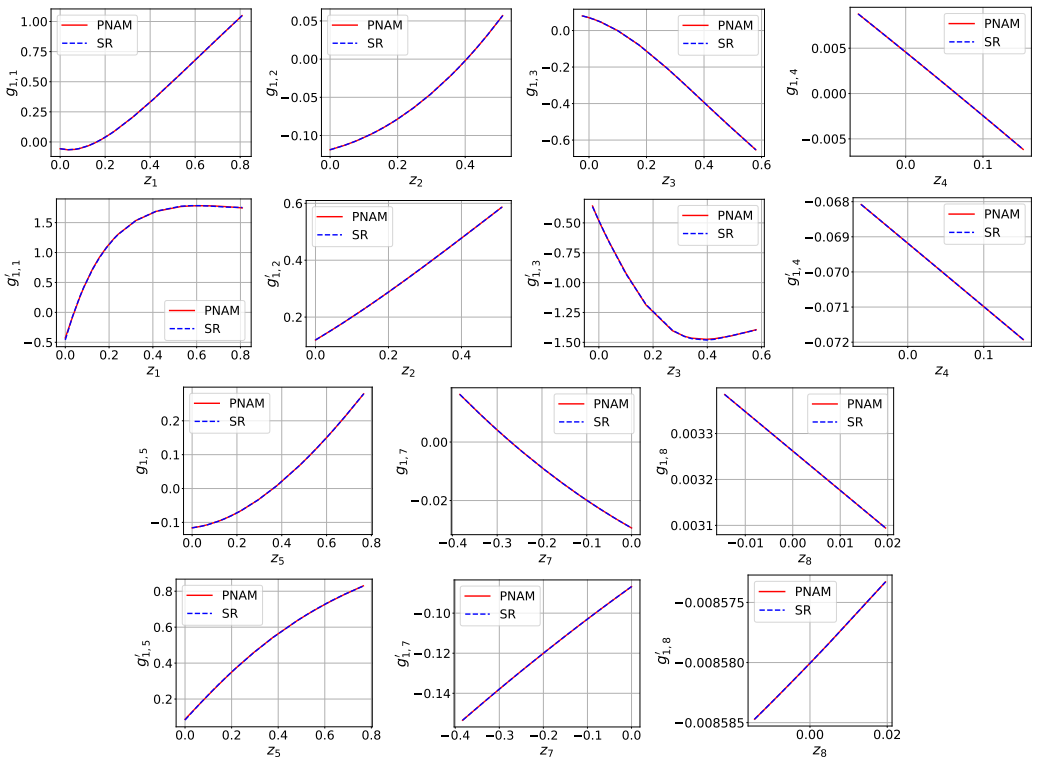


Figure A.4: Bases $\{g_{1j}\}$ and their derivatives. The expressions of $\{g_{1j}\}$ are presented in Table 5.

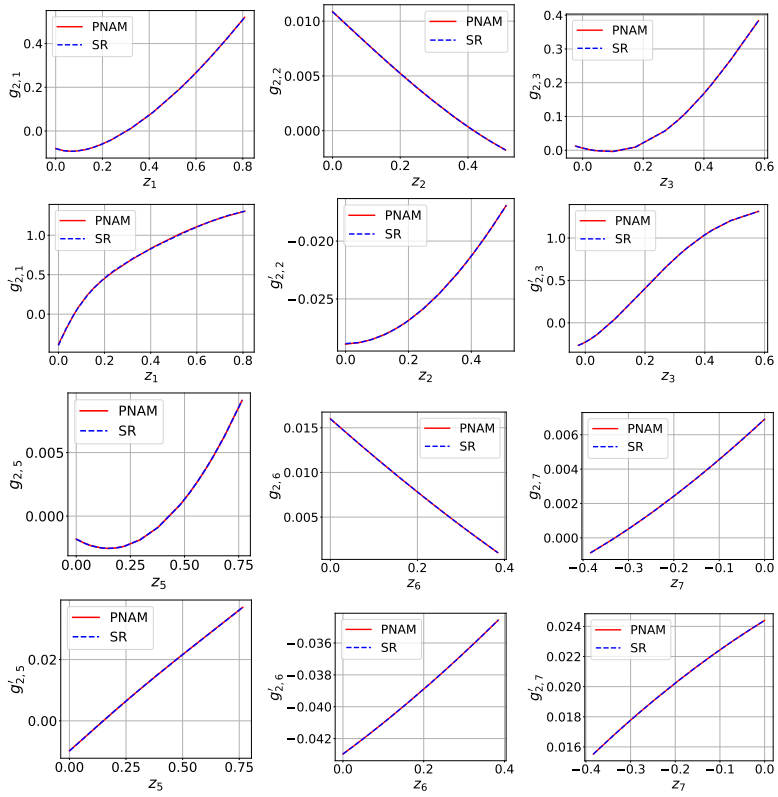
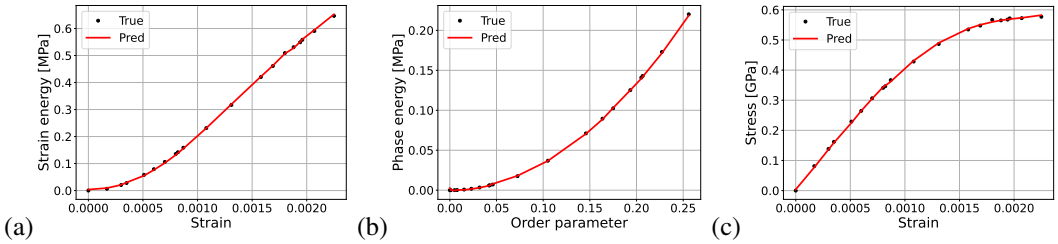


Figure A.5: Bases $\{g_{2j}\}$ and their derivatives. The expressions of $\{g_{2j}\}$ are presented in Table 5.



(a) (b) (c)

Figure A.6: Test predictions for the linear combinations of the polynomials $\{g_{ij}\}$ in Table 5. (a) Linear combination of $\{g_{1j}\}$, (b) linear combination of $\{g_{2j}\}$, and (c) derivative of the sum of the linear combinations of $\{g_{1j}\}$ and $\{g_{2j}\}$ with respect to the strain.