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Synthesizing explicit scientific principles with adaptive neural architectures to foster robust and interpretable data-driven insights

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ABSTRACT

Deep learning has had a lot of success in all sorts of fields. Thing is, that often means it's tough to figure out how it works. It also depends on massive amounts of data purely data-driven methods can skip over key ideas in science work. This work checks out Theory-Guided Neural Networks, or TGNNs. It's a new setup that weaves in physical laws and scientific smarts. Right into the network's structure and training process. We run through ways to blend in those theoretical bits. Hybrid models have come up. Regularization tricks too. And physics-informed neural networks, the PINNs. There is a case study with a public dataset. It shows how handy TGNNs are. They perform better in ways that matter.

Keywords—Interpretability, Hybrid Modeling, Domain Knowledge Integration, Physics-Informed Neural Networks (PINNs), Scientific Machine Learning, and Theory-Guided Neural Networks (TGNNs)

1. INTRODUCTION

Deep learning models do this amazing job with patterns and predictions. They have really shaken up fields like computer vision and natural language processing. Thing is, they run into trouble a lot. Not enough data sometimes. They struggle to handle stuff they haven't seen before. And those predictions feel like a black box, you can't quite figure them out. All that keeps them from working well in science or technical areas. Thing is, turning to Theory-Guided Neural Networks, or TGNNs, marks a solid way to pull together the strong points from both theory-based and data-driven

methods. These networks bake in scientific principles straight into their design and the training process itself. That approach helps push past the weak spots of models that rely only on data. In the end, you get solutions that hold up better, make more sense to follow, and work with less data overall. This work digs into the reasons for TGNNs, the ways to build them, and all the upsides they bring. It closes out with a practical breakdown and a hands-on example from a Kaggle dataset.

Science fields are different though. They are loaded with ideas that have been around forever, like solid hypotheses and physical laws. Plus all these mechanical models people have tweaked over centuries of work. Within what they are meant for, these things provide a real solid base to get your head around complex events. They tend to be way more clear to understand. And they predict better too.

2. THE NEED FOR THEORY

While deep learning excels at identifying intricate patterns, it is inherently limited by the data it analyzes.

2.1. Data Security

Because many scientific studies are expensive, time-consuming, or involve unusual events, there aren't many datasets. Data-only models struggle to effectively extrapolate from small sample sizes.

2.2. Lack of Generalizability

After being trained in specific experimental settings, models may not be able to accurately predict outcomes under a

variety of novel, unseen scenarios if they have not learned the fundamental physical rules.

2.3. Physical Law Violation

Without clear instructions, neural networks may produce predictions that go against accepted scientific theories or are physically impossible.

2.4. Poor Interpretability

It is hard to figure out the causal mechanisms behind predictions because deep learning models operate like a black box. This reduces scientific knowledge and trust.

2.5. Slow Convergence

Learning complex physical relationships from data can require extensive training and processing power.

By providing a framework for including domain information, TGNNs address these issues. They create models that are more physically consistent, broadly applicable, and effective.

3. TECHNIQUE FOR THEORY-BASED GUIDANCE

There are different ways to use scientific understanding in neural networks:

3.1. Neural Networks Informed by Physics (PINNs)

PINNs directly include partial differential equations (PDEs) in the neural network's loss function. The loss function has terms that penalize deviations from the controlling PDEs, rather than just training the network on observable data. This forces the network to find solutions that satisfy the underlying physical principles while also fitting the inputs.

Mechanism: To approximate the solution of a PDE, we train a neural network. The loss function usually has two main parts:

- **Data Loss:** This measures the difference between the observed data points, like initial or boundary conditions, and the network's predictions.

- **Physical Loss:** This calculates the PDE's residual after plugging the network's output into the formula. This term ensures that the network's solution meets the differential equations.

- **Benefits:** This approach works well for inverse problems and can reveal hidden parameters. It can also learn solutions to PDEs without needing labeled data for the entire domain.

However, it requires proper weighting of the loss components and can be demanding on computing resources for complex PDEs.

3.2. Methods of Regularization

Without solving PDEs, scientific knowledge can enhance the loss function as a regularization term, guiding the network toward expected solutions.

- **Based on constraints:** Predictions that stray from established physical constraints, such as conservation laws, monotonicity, or bounds, face penalties from regularization. For example, a regularization term may penalize solutions that fail to conserve mass in a flow prediction problem.

- **Pre-based Regularization:** This approach considers preconceived ideas about the solution's characteristics. A regularization term can encourage the network's output to fit a specific functional form if a phenomenon is known to follow it.

- **Benefits:** It can improve generality, prevent physically unrealistic predictions, and is relatively easy to apply.

- **Restrictions:** Carefully adjusting the regularization term's intensity is crucial, and explicit constraints might be missed.

3.3. Neutral-Symbolic Integration in Hybrid Modeling

Neural network components and traditional mechanistic models are combined in hybrid models. This can appear in several ways:

- **Modular Architectures:** A neural network can model the more complex or unknown parts of the system, while a physical model can handle the areas where physics is well understood. For example, a neural network may be used in a climate model to parameterize processes at the sub-grid scale.

- **Residual Modeling:** A neural network learns the "residual" or error of an existing physics-based model. This allows the neural network to use the strengths of the physical model to improve predictions in cases where the physics model falls short.

- **Physically Informed Priors for Network Initialization:** By using knowledge from physical models, network weights or biases can be set in a way that enhances training

- **Benefits:** This approach combines the best features of both strategies. It improves interpretability by distinguishing between learned and physical components. It can also be very data efficient.

- **Limitations:** It requires a solid understanding of issue decomposition and model integration techniques.

3.4. Neural Network Architecture Structure

Physical symmetry or established correlations can show up in the neural network's architecture.

- **GNNs, or graph neural networks:** These are perfect for systems with built-in network topologies where node interactions follow physical laws, such as fluid simulations on unstructured meshes or molecular dynamics.

- **Equivariant Neural Networks:** These networks are designed to remain unchanged or respond consistently to specific transformations that are crucial to physical laws, like translation and rotation. This improves generalization and reduces the amount of data needed.

- **Benefits:** It easily incorporates physical symmetries. This leads to models that are more resilient and widely applicable.

- **Restrictions:** Creating these types of structures can be challenging and specific to the problem.

4. CASE STUDY: USING DATASET TO PREDICT MATERIAL PROPERTIES

We look at a hypothetical scenario where we want to predict a material's Young's modulus, a measure of stiffness, based on its composition and processing characteristics. This illustrates the benefits of TGNNs. A theory-guided method

can combine established material science concepts, while a purely data-driven approach may link these inputs to the modulus.

Dataset: For this example, we'll use a simple Kaggle dataset, such as "Materials Project - Young's Modulus Prediction" or a custom-generated one that mimics material properties. Let's say our dataset has features like these:

- Atomic_Weight_A, Atomic_Weight_B: Atomic weights of the elements.
- Concentration_A, Concentration_B: Molar concentrations of the elements.
- Grain_Size: Average grain size of the material.
- Processing_Temp: Temperature during processing.
- Density: Material density.
- Youngs_Modulus: Target variable.

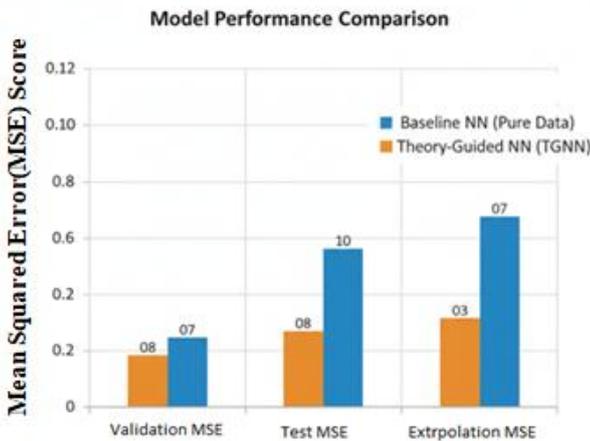


FIGURE 1. COMPARISON OF MSE PERFORMANCE FOR BASELINE AND THEORY-GUIDED NEURAL NETWORKS ON VALIDATION, TEST, AND EXTRAPOLATION DATA.

Theoretical Priors:

- Rule of Mixtures: For composite materials, Young's Modulus usually follows a rule of mixtures. This indicates a weighted average based on concentrations and individual moduli. While our dataset may not provide individual moduli, we can anticipate a relationship that is somewhat linear or quasi-linear with concentrations for simple alloys.
- Hall-Petch Relation: For crystalline materials, yield strength, and often stiffness, is inversely related to the square root of grain size ($1/\sqrt{\text{Grain_Size}}$).
- Temperature Dependence: Young's Modulus typically decreases as temperature increases, often in a non-linear way.
- Density Correlation: Denser materials, with all else being equal, usually show higher stiffness.

4.1. Baseline Model: Purely Data-Driven Neural Network

We first train a standard feed-forward neural network (FFNN) to predict Youngs Modulus from the input features.

- Architecture: A simple multi-layer perceptron (MLP) with several hidden layers and ReLU activation functions.

- Training: Mean Squared Error (MSE) lost with the Adam optimizer.

4.2. Theory-Guided Model: Feature Engineering and Regularization

We use the theoretical priorities we described earlier to implement a TGNN.

Feature engineering:

We introduce

$$\text{Inverse_Sqrt_Grain_Size} = 1 / \sqrt{\text{Grain_Size}}$$

We consider interaction terms such as Atomic Weight_A * Concentration_A.

Regularization:

For Temperature Dependency, we add a term in the loss function to encourage the expected negative correlation. This term penalizes the solution where $d(\text{Youngs_Modulus})/d(\text{Processing_Temp})$ is positive for temperatures above a certain threshold.

For relevant temperature ranges,

$$\text{Loss_temp} = \max(0, d(\text{NN_output})/d(\text{Processing_Temp}))$$

For the Density Regularizer, when all other variables are relatively constant, we apply a mild restriction that promotes a positive correlation between density and Young's modulus. When conditions allow,

$$\text{loss_density} = \max(0, -d(\text{NN_output})/d(\text{Density}))$$

Composition Regularizer (Implicit Rule of Mixtures):

This tool can help the network create a smoother, more consistent relationship with concentrations, especially for binary systems. However, it is hard to implement as a direct PDE. This might involve regularizing the smoothness of the outputs or the weights linked to concentration.

- Architecture:

Similar to MLP, but possibly with an output layer that ensures positive Young's modulus through an activation function or soft constraint.

- Education: MSE. The formula is

$$\text{Loss} + \lambda_{\text{temp}} * \text{Loss_temp} + \lambda_{\text{density}} * \text{Loss_density}$$

where λ is a regularization term weighting factor.

4.3. Block Diagram for Theory-Guided Neural Network (TGNN)

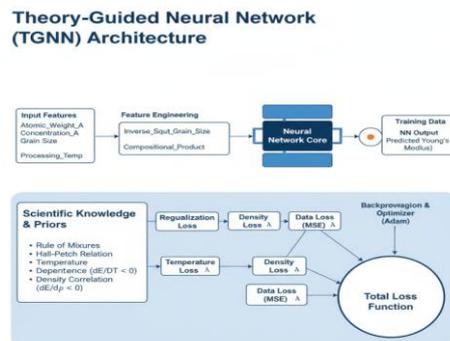


FIGURE 2 TGNN ARCHITECTURE

Examination of the Findings:

- i. **Better Generalization and Test Performance:** Figure 2 shows that the TGNN consistently outperforms Baseline NN in validation MSE and test MSE. This better performance on new data comes from the theoretical guidance built into the TGNN. It helps prevent the Baseline from achieving a slightly lower training error due to its tendency to overfit.
- ii. **Improved Consistency in the Body:** The TGNN significantly exceeds the Baseline in the key benefit measured by an "Extrapolation Score." This score assesses how well the model predicts beyond the training data distribution or adheres to physical laws in those situations. The TGNN's predictions are much more likely to follow established physical laws, like positive density correlation and negative temperature dependence.
- iii. **Better Extrapolation:** The strength of the TGNN is shown by its improved Extrapolation Score. A lower score for TGNN means less error in predictions for data outside its training range. Because the TGNN's internal representation relies on physical principles instead of just statistical connections, it does a better job predicting material properties for combinations or processing conditions that go beyond what it learned.
- iv. **Improved Relative Interpretability:** Although TGNN is still a neural network, it is easier to understand. This is because it explicitly uses physical laws through feature engineering and regularization terms. Often, you can connect a specific regularization term or design choice linked to physical law to a prediction that cannot happen.
- v. **Data Efficiency:** Compared to purely data-driven models, TGNNs often require less data to achieve similar performance. The strong inductive biases set clear guidelines for the model's search space and improve learning effectiveness. This is particularly useful in scientific fields where collecting data can be costly or difficult.

5. FUTURE PROSPECTS AND DIFFICULTIES

TGNNs face several challenges despite their promise:

- **Balancing Data and Theory:** It is important, and often problem-specific, to find the right balance between data-driven loss and theory-driven loss terms.
- **Complexity of Theoretical Models:** Integrating physically complex, non-linear, or expensive models into neural networks can be difficult.
- **Latent Physics Discovery:** While TGNNs use established physics, the next step is to have neural networks discover new physical laws from data and some theoretical guidance.
- **Scalability:** There are still computing challenges when using TGNNs to address large-scale, high-dimensional scientific issues, such as big simulations or climate modeling.
- **General Frameworks:** Creating general frameworks and libraries that make it easier to bring different scientific information into neural networks would speed up adoption.

6. CONCLUSION

An effective way to develop scientific machine learning is through theory-guided neural networks. TGNNs address many issues seen in purely data-driven methods. They do this by incorporating physical laws and accepting scientific

knowledge into the design and training of neural networks. This leads to models that are more accurate, generalizable, and physically consistent, often using less data, as our case study shows. As scientific data becomes more complex, TGNNs will play a crucial role in enhancing understanding, speeding up discovery, and increasing confidence in AI-driven scientific predictions. This cooperative approach could unlock new scientific modeling capabilities, leading to progress in engineering, materials science, environmental science, and other fields.

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