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A physics-informed evolutionary regression framework for constitutive models of soils

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ABSTRACT: Developing accurate constitutive models for soil behaviour is fundamental to predicting ground engineering problems. Several constitutive models have been developed to capture the complex behaviour of soil under various external conditions. Elasto-plasticity-based constitutive models, including Modified Cam Clay, NorSand, and bounding surface models, are well-known examples widely used in geotechnical projects. However, the new models often include additional parameters that must be determined through extensive laboratory testing and calibration procedures. Increasing model complexity also makes numerical convergence more challenging. Machine learning (ML) constitutive models, on the other hand, can offer practical solutions for complex geomaterial modelling. Such approaches can predict the history-dependent behaviour under various loading conditions. Models are directly developed from available data using experiments or simulations predicting soil behaviour. ML-based material models, in their standard form, however, have limited predictability and accuracy outside their training range due to the absence of underpinning physics, such as thermodynamic laws, which reduces their applicability in real-world scenarios. Incorporating thermodynamic constraints into the learning process can enhance the robustness and reliability of models, even for data beyond the training range. In recent years, physics-based neural network frameworks have been introduced to address some of the above problems. They are, however, typically black-box models, leading to a lack of physical interpretability, and their complex network architectures, often with many parameters, further reduce computational efficiency. This research proposes a novel approach for constitutive modelling based on a physics-informed evolutionary regression (PIER) method to predict nonlinear sand behaviour under various stress paths. PIER can produce interpretable mathematical models that enhance computational efficiency and ensure thermodynamic consistency in predictions for both observed data and unseen scenarios that may extend beyond the training range. Results demonstrate the applicability of PIERs for predicting contractive behaviour of sand.

KEYWORDS: Data-driven computational mechanics, Physics-Informed Machine Learning, Interpretable data-driven model, Constitutive model.

1 INTRODUCTION

Elastoplastic theories explain soil behaviour by combining a reversible model and an evolved yield function (Kolymbas, 1991). These models often require extensive laboratory testing and calibrations to determine additional parameters and to develop a mathematical function representing all possible soil behaviours. (Haghighat et al., 2023). The complexity of these models also makes numerical convergence more challenging (Dong, 2023). In the past two decades, the use of machine learning (ML)-based constitutive models has been an alternative for reducing computational burden in material modelling. This approach predicts soil history-dependent behaviour under different loading conditions (Masi et al.,2021). ML-based material modelling dates back to the 90s when Ghaboussi et al. (1991) proposed an artificial neural network (ANN)-based constitutive model for concrete. Although ML models such as ANNs can provide well-fitting observations, some cannot extract interpretable knowledge from massive datasets. It is also possible to encounter physical inconsistency, such as the inability to follow thermodynamic laws to make accurate predictions based on data not part of the learning process. To overcome these challenges, physics laws can be incorporated into ML processes, leading to the so-called physics-informed neural network (PINN) method (Raissi et al., 2019). Thermodynamic-based neural networks (TANNs) were proposed by Masi et al. (2021) for modelling rate-independent elastoplastic materials with inelastic behaviour. Many researchers have applied the NN methods to accurately track yield surface loci in ML-based models (Bahmani et al., 2023; Haghighat et al., 2023; Vlassis & Sun, 2021; Weber et al., 2023), a challenging task when multiple processes are involved. Additionally, they are typically viewed as black-box models, lacking explicit input-output relationships. This impacts physical interpretability and computational efficiency.

By using ML methods based on evolutionary algorithms and symbolic regression, explicit formulations can be developed for material modelling that are interpretable. This paper proposes a novel physics-informed evolutionary regression (PIER) to model sand's stress-strain and volumetric behaviours. The PIER proposes thermodynamically consistent and interpretable constitutive laws, which do not rely on tracking yield surface loci. Predictions are compared with actual data, and results demonstrate the robustness and extrapolation capabilities of the PIER. For simplicity, thermal processes and other thermodynamic variables have been omitted.

2 THERMODYNAMIC CONSTRAINTS

The principle of non-negative dissipation plays a key role in solid mechanics, and constitutive relationships must comply with the thermodynamic laws, governing energy conservation (Puzrin, 2012). If the model satisfies the second law of thermodynamics (Dornheim et al., 2023), it can be considered thermodynamically consistent. This law states that the dissipation rate, which reflects the level of disorder or randomness in a system, must always be non-negative (Ziegler & Wehrli, 1987). In boundary value problems (BVPs), this phenomenon may influence the accuracy of predictions and compatibility with universal laws for plastic deformations, such as surface settlements (Masi et al., 2021). In this research, by integrating the law as a constraint into the ML structure during the learning process, the robustness of physically consistent solutions for BVPs in geomechanics is enhanced. Equation (1) shows the rate of dissipation density ($\dot{W}^p$), derived from the inner product of stress (σ) and plastic strain rate (D^p). Details of plastic strain rate calculation are provided in (Wu & Niemunis, 1996).

$$\dot{W}^p = \sigma : D^P \quad (1)$$

3 METHODOLOGY

The concept of the proposed methodology is based on combining symbolic regression, evolutionary computing, and the integration of underpinning physics (in this case, thermodynamic laws) to develop an explicit formulation that describes materials' behaviour. Previous studies combining evolutionary regressions, e.g. evolutionary polynomial regression (EPR) (Giustolisi & Savic, 2006), have been used to model various phenomena, including predicting the behaviour of geomaterials. In general, such data mining techniques identify the best polynomial equation with the typical formulation of $y = \sum_{j=1}^{m} F\left(X, f(X), a_j\right) + a_0$, that fits the data by combining a genetic algorithm (GA) and a least squares (LS) method. Where y is the predicted output, F and f are functions defined by the process and the user, respectively; X is the input matrix; a_j and a_0 are constant parameters estimated and bias, respectively. Some of the successful applications of the EPR include modelling the liquefaction potential of sand (Gue et al., 2021), assessing the behaviour of soil under cyclic loading (Javadi et al., 2012), and predicting the stress-strain behaviour of materials (Javadi & Rezania, 2009). Faramarzi et al. (2012) have developed an EPR-based material model assessing the volumetric behaviour of soils.

The proposed approach in this research is physics-informed evolutionary regression (PIER), an ML framework that integrates thermodynamic laws to improve extrapolation capability. Figure 1 illustrates the proposed PIER-based material modelling to derive a constitutive model to capture the plastic behaviour of sands, which is thermodynamically consistent. This process represents an iterative approach, finding a mathematical equation. GA optimises exponents and searches for the symbolic structure of the equation, and LS estimates coefficients. During the optimisation process, a thermodynamic constraint is integrated into the learning process.

Unlike elasticity, current stress cannot be obtained from current strain (Kolymbas, 1991; Mašín, 2019), so stress is defined as a function of the entire deformation history, i.e. strain and strain rate, $\sigma = f(\varepsilon, \dot{\varepsilon})$. Stress can be expressed as a polynomial form with unknown coefficients and exponents, where n is the number of terms in a polynomial expression, a_i are coefficients, and α, β are exponents.

$$\sigma = \sum_{i=1}^{n} a_i \left(\varepsilon_1^{\alpha_{1i}} \dot{\varepsilon}_1^{\beta_{1i}} \varepsilon_2^{\alpha_{2i}} \dot{\varepsilon}_2^{\beta_{2i}}\right) + a_0 \tag{2}$$

An initial trial-and-error process was carried out, which led to the exponents and number of terms in the equation being restricted to the range [0, 1, 2] and five, respectively. The PIER approach imposes the thermodynamic requirement of energy dissipation ($\dot{W}^p \geq 0$) on the GA's objective function, leading to more reliable solutions for various stress paths.

Coefficients of determination (CoD) are used to determine the accuracy of each stage, where y_o, y_p, and N are the vector of observed data, the predicted value, and the number of observations, respectively.

$$CoD = 1 - \frac{N-1}{N} \frac{\Sigma_N \left[(y_p - y_O)^2\right]}{\Sigma_N \left[\left(y_O - \frac{1}{N}\Sigma_N y_O\right)^2\right]} \tag{3}$$

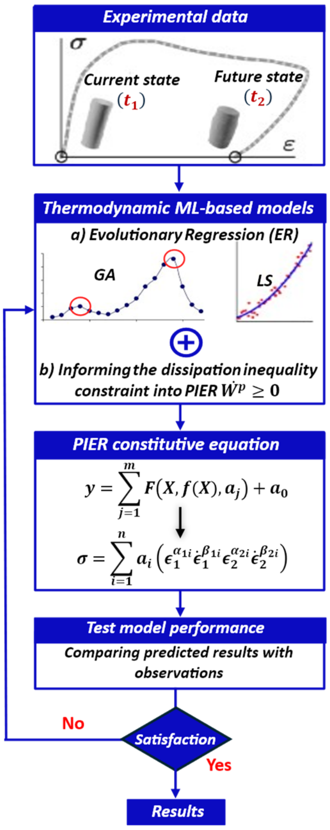


Figure 1. Schematic of the PIER-based material model.

3.1 *Data preparation*

The results from a series of monotonic drained triaxial tests for Karlsruhe sand are used to demonstrate PIER's capability to describe the behaviour of soil (see Table 1). There are five effective confining pressures, including $\sigma_3' = p'_0 = 50$, 100, 200, 300, and 400 kPa. Also, the initial relative density I_{D0} ranges from 0.15 to 0.25. 80% and 20% of the dataset were used for training and validation, respectively (Wichtmann & Triantafyllidis, 2016).

Table 1. A series of drained monotonic triaxial tests.

Test number	p'_0(kPa)	$e_0\ (-)$	$I_{D0}\ (-)$
CD1	50	0.996	0.15
CD2	100	0.975	0.21
CD3	200	0.975	0.21
CD4	300	0.970	0.22
CD5	400	0.960	0.25

Initial effective mean pressure p'_0, void ratio e_0 and relative density I_{D0}.

4 RESULTS AND DISCUSSION

4.1 *Drained triaxial compression tests*

Simulations of drained monotonic triaxial tests were performed with various initial confinement pressures ($50 \leq p_0 \leq 400$ kPa) and relative densities ($0.21 \leq I_{D0} \leq 0.25$). PIER models are trained with initial confinement pressures of 50, 200, and 400 kPa in CD1, CD3, and CD5. Tests CD2 and CD4, with initial confinement pressures of 100 and 300 kPa, are used to validate the PIER models.

As a result of the training and testing procedures, the best PIER equations for axial stress PIER-σ_1 and radial stress PIER-

σ_2 are selected. Table 2 shows the equations, where ε_1 and ε_2 represent the axial and radial strains, respectively, $\dot{\varepsilon_1}$ and $\dot{\varepsilon_2}$ are their corresponding strain rates, p'_0 is the initial effective confinement pressure, and a_i are coefficients. The equations represent constitutive material models for Karlsruhe sand. In these models, CoD values represent the level of accuracy in axial and radial stresses, and CoDs for the training and validation data are 99.98% and 99.93%, respectively.

Table 2. PIER-based equations for Karlsruhe sand under varying loading conditions and relative density.

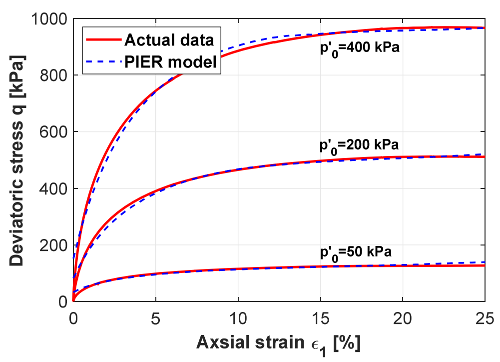
Label	Constitutive equation
PIER-σ_1	$a_0 + a_1\,\varepsilon_2\,\dot{\varepsilon_1}\,p'_0 + a_2\,\varepsilon_1\dot{\varepsilon_1}^2 p'_0 + a_3\,p'_0 + a_4\,\varepsilon_1\dot{\varepsilon_1}^2 p'^2_0$
PIER-σ_2	$a_0 + a_1\,\dot{\varepsilon_1}\dot{\varepsilon_2}\varepsilon_2^2 + a_2\,p'_0 + a_3\,\varepsilon_1\dot{\varepsilon_1}^2 p'_0 + a_4\,p'^2_0$

$^*a_0$ = -15.4, 0.75, $^*a_1$ = 154.84, 151,4, $^*a_2$ = -84.45, 1.00
$^*a_3$ = 1.33, 0.03, $^*a_4$ = -0.012, -1.7 × 10^{-5}

Figures 2 to 4 compare the models' predicted values with the experimental data, highlighting PIER's predictive accuracy and extrapolation capability.

In Figure 2 the stress-strain $(q - \varepsilon_1)$ predicted by PIER are compared to the experimentally measured values for the training and testing datasets. Solid lines demonstrate results from actual data, while dashed lines represent the PIER model's predictions. From these figures, it is evident that PIER-based models can accurately reproduce stress–strain curves. This demonstrates the model's ability to capture the soil's critical state behaviour. Furthermore, the models were used to calculate volumetric behaviour by solving equation PIER-σ_1 in Table 2. The results are shown in the volumetric space $(\varepsilon_1 - \varepsilon_v)$ space in Figure 3.

(a)



(b)

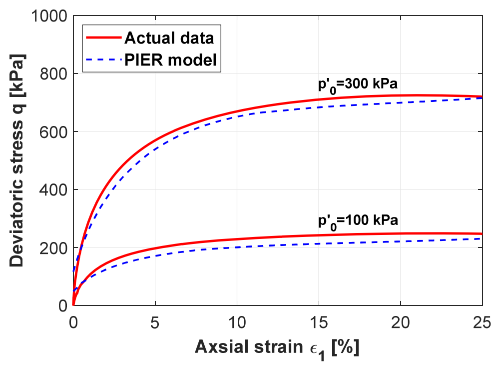
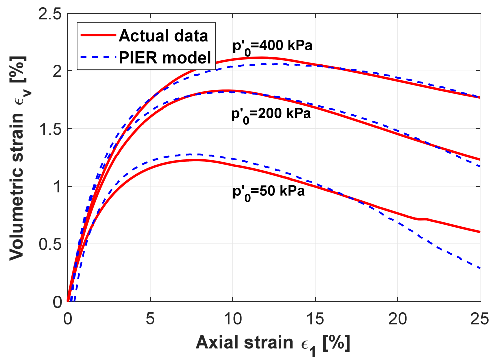


Figure 2. Comparison of the PIER predictions against triaxial tests on deviatoric stress versus axial strain, **(a)** training, **(b)** validation.

(a)



(b)

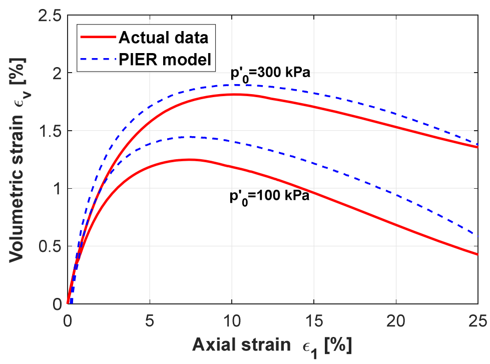


Figure 3. Comparison of the PIER predictions against triaxial tests on volumetric strain versus axial strain, **(a)** training, **(b)** validation.

It can be seen that the PIER model has successfully captured the overall behaviour and trend of the soil response under different confining pressures. It has also reproduced key features of the contractive behaviour of sand under varying density conditions (See Figure 3).

4.2 *Extrapolation capability of the PIER for stress-strain behaviour*

Combining thermodynamic laws as constraints into the learning process can enhance the robustness of the model's predictions for data points beyond the training range. To evaluate the extrapolation capability of the PIER-based constitutive equation, its performance is compared against other models, including a non-physical constitutive model. Equation ((4) illustrates the axial stress in the pure-ML model with a CoD of 99% for both training and testing, where $a_0 = -22.96$, $a_1 = 157.10$, $a_2 = 79.08$, $a_3 = 0.98$, and $a_4 = 0.015$.

$$\sigma_1 = a_0 + a_1\,\varepsilon_2\,\dot{\varepsilon_1}\,p'_0 + a_2\,\varepsilon_1\dot{\varepsilon_1}p'_0 + a_3\,p'_0 + a_4\,\varepsilon_1\dot{\varepsilon_1}\,p'^2_0 \quad (4)$$

The performance of the prediction is evaluated under an initial confining pressure of 500 kPa, a condition that falls outside the training dataset. As shown in Figure 4, the stress-strain curve of the PIER-σ_1 is compared to the ML-σ_1 model. The stress-strain curve in the PIER closely matches the experimental trend; however, in the pure-ML, it deviates after 5% axial strain level. Therefore, due to the absence of the thermodynamic constraint in the latter model, stress-strain behaviour is predicted inappropriately.

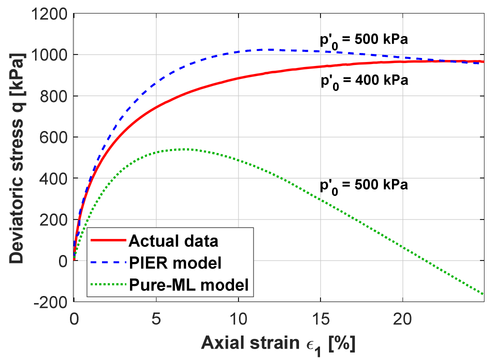


Figure 4. Comparison of the extrapolation capability of the PIER and the pure-ML model for the stress-strain curve.

5 CONCLUSION

This research proposes an approach for developing a physics-informed evolutionary regression (PIER) to capture the behaviour of sandy soils. This model developed a constitutive material modelling, which is interpretable and thermodynamically consistent. The PIER model is trained and validated using experimental data from drained monotonic triaxial compression tests on fine sand samples across a wide range of densities and confinement pressures.

Key advantages of the proposed approach are as follows:

- Combining the thermodynamic law with the ML process enhances the reliability and robustness of predictions in extrapolation scenarios.
- PIER developed interpretable equations that reflect meaningful stress-strain relationships, compared to the black-box neural network models. Mathematical expressions also improve computational efficiency and physical interpretability.
- The level of accuracy (CoD) in the developed equations represents the capability of the PIER in predicting contractive behaviour of the soil.
- PIER-based material modelling is not reliant on tracking yield surface loci.

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