



UNIVERSITY OF TÜBINGEN
COMPUTER SCIENCE DEPARTMENT

Evaluating Machine Learning Models for Modelling Piezo Dynamics

Researchproject Report

Author
David KLEINDIEK

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1 Introduction

1.1 Motivation

The semiconductor industry is concerned with the development and manufacture of semiconductor components. These components are at the heart of many modern systems, from computers and cell phones to vehicles and medical devices. It is a constantly evolving field that is moving towards ever smaller and more complex structures. Today's structure sizes are less than 10 nm, which is about one ten-thousandth of the diameter of a hair.

Failure analysis (FA) of such small structures is a highly specialized task that requires both skilled operators and highly accurate and reliable probing systems, but is essential after design and manufacturing. FA technology continues to evolve toward systems that provide even higher positioning accuracy and longer time of contact (TOC). This requires constant mitigation of the effects that prevent the system from achieving state-of-the-art results.

Central to achieving these advanced FA capabilities is the precise and reliable control of piezoelectric actuators (piezos), which are commonly used in probing systems. These actuators provide the delicate manipulation required to interface with small semiconductor structures. However, their inherent nonlinear behaviors - hysteresis and creep - pose significant obstacles to achieving the high positional accuracy and extended TOC required for modern FA. Hysteresis introduces positional uncertainty due to the dependence of displacement on voltage history, while creep leads to gradual drift even under constant voltage. Together, these effects undermine the reproducibility and efficiency of critical test procedures, limiting the overall effectiveness of the FA process.

1.2 Problem statement

Traditional approaches to mitigating piezo hysteresis and creep often rely on separate mathematical models, each designed to treat one phenomenon in isolation [1–3]. This fragmented approach fails to capture the coupled dynamics and complex interplay between hysteresis and creep observed in real-world applications. While some models attempt to incorporate the underlying physics, their effectiveness is often limited by the intricate nature of these phenomena. The resulting need to develop and tune multiple models is cumbersome and can lead to suboptimal performance in practice. In addition, the parameter tuning required for these individual models is often extensive and may not generalize well across different operating conditions or piezo actuator types. Each system exhibits unique dynamics and a distinct "fingerprint" that is difficult to capture with traditional models. This highlights the need for a unified modeling approach that can simultaneously account for both hysteresis and creep, while effectively capturing the unique characteristics of individual systems.

This study aims to use machine learning (ML) techniques to develop a novel, unified model of piezo behavior. We hypothesize that data-driven ML models, trained on the recorded behavior of individual systems, can capture the complex nonlinearities and unique dynamics of piezos more effectively than traditional approaches. By learning the specific "fingerprint" of each system, the ML models can provide a highly accurate estimate of its behavior. The performance of well-established ML techniques such as linear regression, basic neural networks, and long short-term memory (LSTM) networks, as well

as state-of-the-art Kolmogorov-Arnold networks (KANs) will be evaluated.

By comparing these different ML approaches, we aim to identify the most promising models for accurately predicting piezo hysteresis and creep in the context of semiconductor failure analysis. We expect that the findings will not only advance the understanding of piezo behavior, but also pave the way for the development of more robust and intelligent piezo control systems. These advances could significantly improve the reliability and efficiency of semiconductor testing, ultimately benefiting the broader field of electronics manufacturing.

2 Background Nanoprobing

Nanoprobing is a technique from the field of nanoelectronics that is used to analyze components in the nanometer range. The technique uses special measuring tips to interact with nanoscale structures and determine their electric properties. An important field of application in the semiconductor industry is the fault analysis of transistors. Electrical faults such as short circuits, interruptions, resistances and leakage paths are detected and analyzed. Kleindiek Nanotechnik (KN) manufactures devices and measurement electronics for nanoprobing and is a world leader in this field [4]. For a detailed explanation of nanoprobing and an insight into the company Kleindiek Nanotechnik, please refer to the video by Roman Hartung [5, 6].

2.1 Nanoworkstation

KN has developed the Nanoworkstation, the system can be equipped with multiple manipulators. Each manipulator can be moved in three axes: A for left/right, B for up/down, C for in/out. By using a specially developed piezo motor, the manipulators operate in the sub-nanometer range and allow precise physical manipulation and characterization of electrical and material properties in the micro- and nanoscale.

2.2 Micromanipulator

The Kleindiek Nanotechnik MM3E used for this study is a high-precision, closed-loop micromanipulator system designed for demanding nanoprobing applications [4]. It is equipped with position encoders on all axes, allowing precise localization of the probe tip with a resolution of $1\text{ }\mu\text{m}$ in the a and b axes and 70 nm in the c axis.

For this study, a modified version of the MM3E was used to push the limits of encoder resolution to fully capture the subtle effects of creep and hysteresis, at the cost of increased noise in the sensor readings. The modified MM3E encoders achieves a resolution of 250 nm in the a and b axes and 20 nm in the c axis, providing the sensitivity necessary to detect and quantify even minute creep-induced displacements.



Figure 1. A Nanoworkstation from KN, equipped with four Micromanipulators.



Figure 2. A MM3E Manipulator from KN with a rotating tip attachment.

2.3 Piezoelectric Actuators

Piezoelectric actuators, often referred to simply as "piezos," are a core technology that enables the precise motion required in nanoprobeing. These actuators exploit the piezoelectric effect, a phenomenon in which certain materials (piezoelectric ceramics or crystals) change shape in response to an applied electric field [7].

When a voltage is applied to a piezoelectric material, its internal crystal structure is distorted, resulting in a macroscopic change in shape. This deformation is typically on the order of microns or less, making piezos ideal for fine positioning applications such as those found in nanomanipulators.

The MM3E described in section 2.2 uses piezos to drive the movement of its probe tip along each axis (a, b, and c). These actuators are typically controlled by a voltage range of -80 V to 80 V , allowing both extension and contraction of the piezo material, and thus precise bi-directional movement of the probe.

While piezo actuators offer numerous advantages, they also present certain challenges that must be addressed for optimal nanoprobe performance.

2.4 Hysteresis

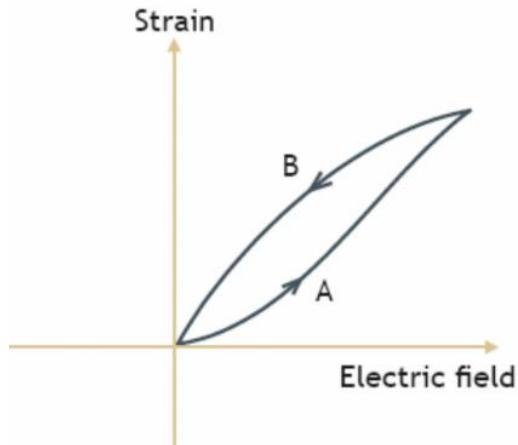


Figure 3. Example hysteresis curve of a piezo.

Source: noliac [8]

Hysteresis, a pervasive phenomenon in piezos, manifests itself as a rate-independent non-linearity between the applied voltage and the resulting displacement. It exhibits a dependence on both the current and past applied voltages, giving it a memory-like behaviour. This nonlinearity results from the complex interplay of several factors inherent in the ferroelectric nature of the material. The hysteresis effect poses a significant challenge in applications that require precise positioning, such as nanoprobeing. It introduces positional uncertainties and errors due to the path-dependent nature of the displacement-voltage relationship. In open-loop operation, hysteresis can introduce significant positioning errors, sometimes reaching 10-15% of the actuator's operating range [9]. This makes it difficult to accurately predict the final position of the piezo actuator based on the applied voltage alone.

2.5 Creep

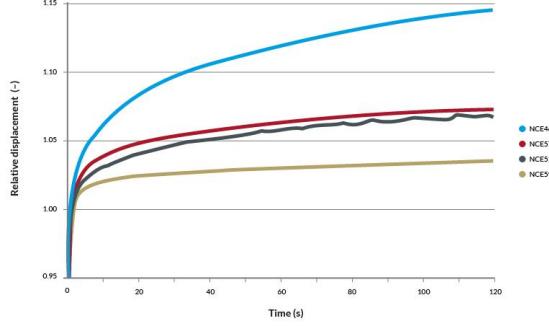


Figure 4. Creep characteristic for different piezo materials.

Source: noliamc [8]

This phenomenon manifests itself as a slow drift in the displacement of a piezo after the application of a voltage step. It is primarily attributed to the gradual relaxation of internal stresses and changes in the residual polarization of the piezo material. Creep becomes increasingly problematic over longer periods of time, resulting in a deviation from the desired position [10, 11]. This is particularly critical in applications such as semiconductor probing, where maintaining precise contact between the probe (driven by the piezo) and the sample over long periods of time is essential. Even a small amount of creep drift can result in loss of contact with the target structure, interrupting the measurement or even causing damage. While operating the piezo at higher frequencies can partially mitigate creep, it remains a persistent challenge in scenarios where sustained positioning accuracy is required, such as the delicate probing of semiconductor devices.

By understanding and predicting the creep behaviour of the manipulator, we can develop strategies to compensate for this drift, leading to improved positional accuracy, stability and reproducibility in nanoprobe. This, in turn, can improve the reliability and efficiency of semiconductor failure analysis and contribute to advances in nanotechnology research and development.

3 Background Models and Feature Engineering

This section provides an overview of the machine learning models and feature engineering techniques used in this study to predict hysteresis and creep behaviour of piezos.

3.1 Neural Networks

Neural networks are a class of machine learning models inspired by the structure and function of biological neural systems. They consist of interconnected nodes (neurons) organised in layers. Each connection between neurons has an associated weight, and learning occurs by adjusting these weights based on training data [12].

Vanilla NNs can model complex non-linear relationships, making them suitable for capturing the intricate behaviour of piezo actuators. In this study, we will explore different NN architectures and activation functions to find the optimal configuration for hysteresis and creep prediction.

3.2 Long Short Term Memory

LSTM networks are a special type of recurrent neural network (RNN) designed to overcome the vanishing gradient problem that can hinder learning in traditional RNNs [13]. LSTMs introduce memory cells and gates that allow the network to selectively retain or forget information over time. This makes LSTMs particularly well suited to modelling sequential data, where the current output depends not only on the current input, but also on past inputs. [14]

Given the time-dependent nature of creep and the history-dependent nature of hysteresis, LSTMs are a promising candidate for capturing the dynamic behaviour of piezo actuators. We will investigate different LSTM architectures and hyperparameters to optimise their performance for this task.

3.3 Kolmogorov Arnold Network

Inspired by the Kolmogorov-Arnold representation theorem, Kolmogorov-Arnold networks (KANs) offer a promising alternative to traditional multi-layer perceptrons (MLPs). Unlike MLPs, which use fixed activation functions at the nodes, KANs use learnable activation functions at the edges connecting the nodes. This key difference enables KANs to achieve comparable or superior accuracy to MLPs with significantly fewer parameters, demonstrating a faster neural scaling law. This increased interpretability makes KANs valuable tool to uncover and interpret hidden system dynamics. [15] Given their potential advantages in both accuracy and interpretability, KANs are being explored as a powerful tool for modelling complex nonlinear systems, including the hysteresis and creep behaviour of piezo actuators.

3.4 Lasso Regression

Lasso regression, short for Least Absolute Shrinkage and Selection Operator, is a linear regression technique that incorporates regularisation to prevent overfitting and promote sparsity in the model. It does this by adding a penalty term to the standard linear regression loss function that is proportional to the absolute value of the model coefficients.

This penalty term encourages the model to shrink the coefficients of less important features towards zero, effectively performing feature selection. [16]

In the context of modelling piezo hysteresis and creep, lasso regression can be used as a feature selection method to identify the most relevant input features (e.g. past voltage values, step size) for predicting the displacement of the actuator. By identifying and retaining only the most informative features, lasso regression can help simplify the model, improve its interpretability, and potentially improve its generalisation performance to new data.

While lasso regression itself may not be the most powerful model for capturing the complex nonlinearities of piezo behaviour, it serves as a valuable tool for preliminary feature selection. The insights gained from lasso regression can then be used to design and train more sophisticated models such as neural networks, LSTMs or KANs, potentially improving their efficiency and accuracy by focusing on the most relevant features.

3.5 Optuna

Optuna is an open source hyperparameter optimisation framework that automates the process of finding the optimal set of hyperparameters for a given machine learning model. It uses a combination of Bayesian optimisation and evolutionary algorithms to efficiently search the hyperparameter space [17].

In this study, we will use Optuna to tune the hyperparameters of our neural networks, LSTMs and KANs to ensure that we get the best possible performance from each model. This will allow us to fairly compare the different approaches and identify the most promising model for predicting piezo hysteresis and creep.

4 Methodology

This section describes the methods used to create a data set that captures the complex behavior of hysteresis and creep in piezo actuators. It outlines the data collection process, as well as the pre-processing and feature engineering techniques employed.

4.1 Data collection

A comprehensive and meaningful dataset is essential for training effective machine learning models. The dataset developed in this study must meet several criteria:

- **Hysteresis Capture:** The dataset needed to include a wide range of motion patterns with varying hysteresis intensities to ensure that piezo behavior is captured across its full range of motion.
- **Creep Capture:** The dataset required recordings of multiple scenarios with different historical piezo control histories to capture creep behavior under different conditions and positions.

4.1.1 Encoder Noise Quantification

The piezo input voltage is adjusted to different values over the full range (-80 V, -40 V, 0 V, 40 V, and 80 V) and the system is allowed to stabilize at each position for 3 minutes. The encoder readings are then zeroed and the following values are recorded for 20 seconds at the maximum sampling rate of 11 readings per second.

This approach allows quantification of the encoder noise at different displacement of the piezo. By analyzing the fluctuations of the encoder readings around the zeroed position, we can characterize the noise distribution. This information is crucial for understanding the limitations of the sensor data and for validating the machine learning models.

Figure 5 shows the distribution of these encoder readings, which encapsulates the inherent noise in the measurement system. The observed pattern appears to be Gaussian, characterized by a standard deviation (σ) of 20.79 nm. This suggests that most of the noise variation is within this specific range, highlighting the noise level of the enhanced encoders introduced through their higher resolution.

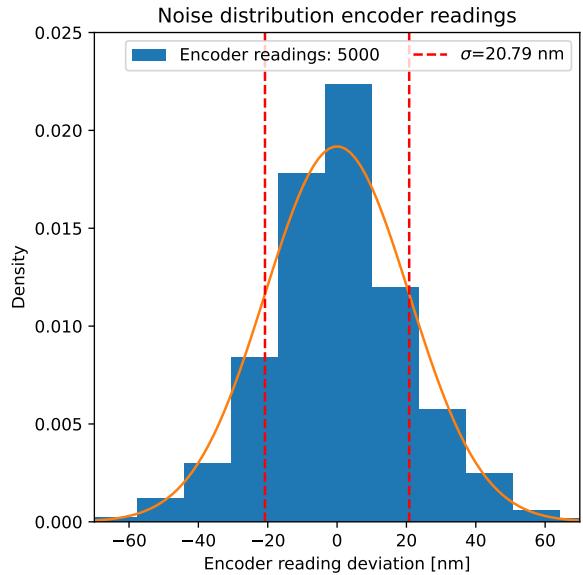


Figure 5. Distribution of the positional deviation of the encoders readings. The underlying distribution is Gaussian with a σ of 20.79 nm

4.1.2 Modified Random Walk

To automate data collection over extended periods of time, a custom random walk algorithm is used to control the input voltage applied to the piezo actuator. This algorithm operates within the limits of $[-80 \text{ V}, 80 \text{ V}]$. A tendency to trend in one direction over longer periods of time is introduced. This results in voltage patterns that covered the entire applicable range, including high peaks and deep valleys, as well as slow and fast motion. In addition, adjustable pause intervals and durations were included to allow recording of creep behavior after specific voltage sequences.

4.1.3 Hysteresis

To gain a deeper understanding of the behavior of the piezo, the voltage range was divided into fractions and the voltage was swept up and down from different starting points. This approach allows the observation of hysteresis effects under different voltage ranges, as shown in Figure 7. In addition, Figure 7 shows the effect effect of the voltage step size on the hysteresis behavior. The full voltage range is swept with different voltage step sizes (from 0.01 V to 1.25 V).

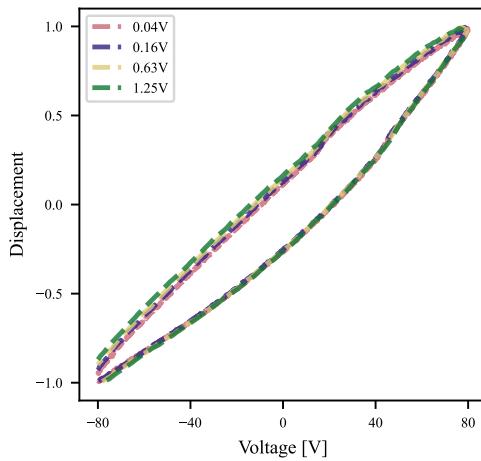


Figure 6. Hysteresis behavior of piezo at different voltage step sizes

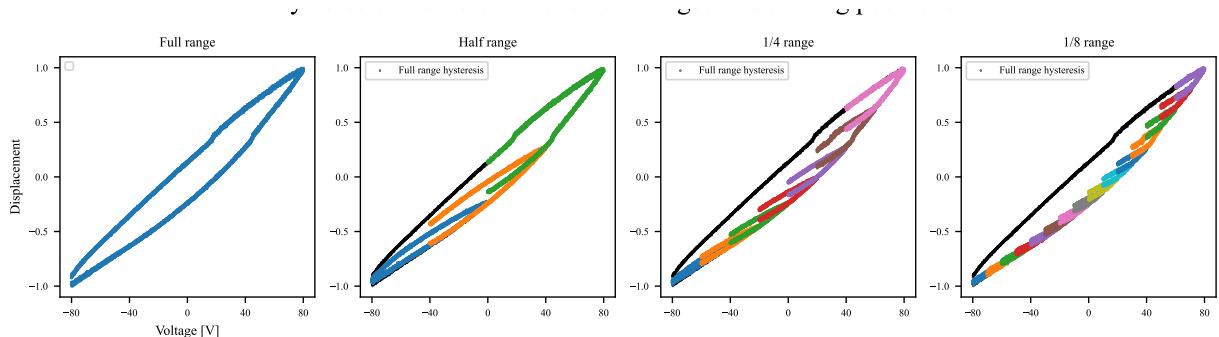


Figure 7. Hysteresis behavior of piezo at different sweep ranges.

Using the modified random walk algorithm, three voltage time series were generated to record a data set for training, evaluating, and testing the models. These sequences were applied to the piezo motor while simultaneously recording encoder readings from the

manipulators to capture the resulting displacement. A dataset containing over 26 hours of recorded data is created this way. A fraction is shown in Figure 8.

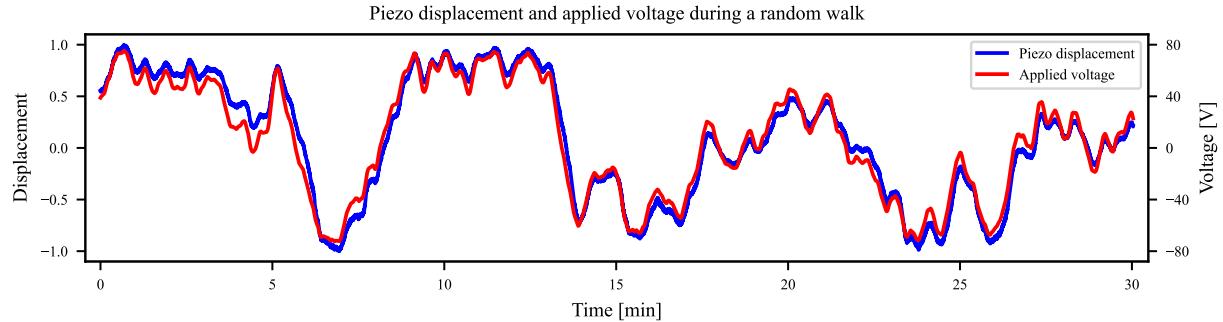


Figure 8. Example of a voltage sequence and recorded piezo displacement that is used to capture hysteresis effects of the piezo.

4.1.4 Creep

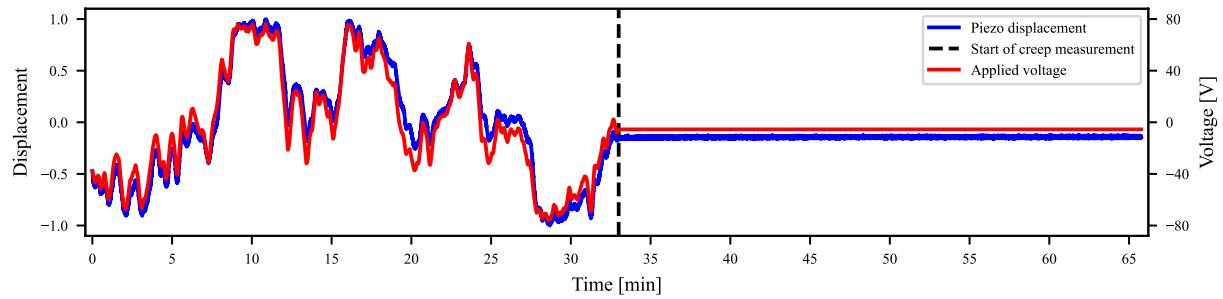


Figure 9. Example of a voltage sequence and recorded piezo displacement that is used to capture creep effects of the piezo.

For effectively capturing the creep behaviour of the piezo under varying conditions, a total of 15 voltage sequences are generated, each is ~ 30 minutes long. After the voltage sequence is applied to the piezo, the voltage is held constant for the following ~ 30 minutes and the resulting creep is measured. Figure 9 shows one of the sequences that is used. In Figure 10 the resulting drift is shown for the different sequences. With a maximum possible displacement of $\sim 2 \mu\text{m}$ The piezo displacement after 30 minutes deviates by up to 10% from the starting position.

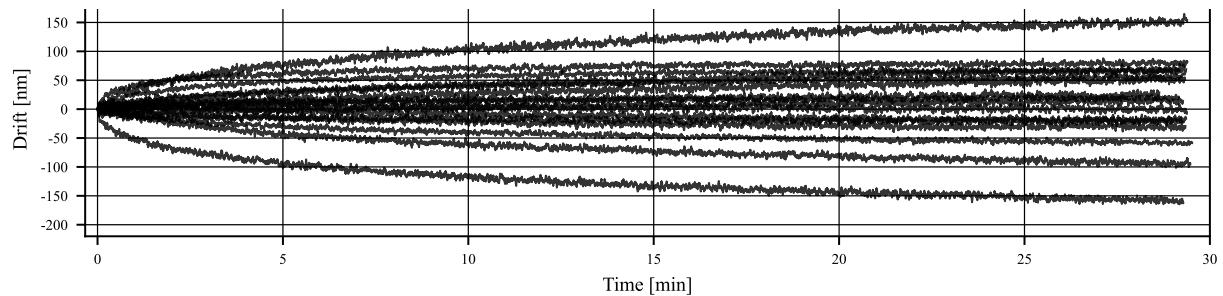


Figure 10. Recorded piezo creep for 15 different histories of applied voltages.

4.2 Feature Engineering

Hysteresis and creep are time-dependent phenomena. Their effects decrease with time after the last voltage step applied to the piezo. The magnitude of these effects is also influenced by the amount of displacement of the piezo, opposite movements can partially cancel each other out.

To capture these complex dependencies, a number of features are developed from the raw data:

- **Lagged Positions:** Past positions of the piezo actuator were included as features, since the current position is influenced by its recent motion history.
- **Last Voltage Step:** The magnitude and direction of the last voltage step are included, as this directly affects the instantaneous hysteresis and creep response.
- **Summed Past Steps:** The cumulative sum of past voltage steps with different window sizes is included, reflecting the overall history of motion and its potential influence on the current state.
- **Rolling Exponential Sums:** Multiple rolling exponential sums of past voltage steps are calculated, giving more weight to recent steps and less weight to older steps. This accounts for the fading effect of hysteresis and creep over time.

This rich set of features aims to capture the intricate relationship between voltage input, time, and piezo displacement, providing a comprehensive representation of the underlying dynamics.

4.2.1 Feature Selection

Lasso regression as described in Section 3.4 is used to identify the most dominant features from this large set. This step is critical for simplifying the later trained models, improving its interpretability, and potentially improving its generalization performance to new data.

The lasso regression analysis identified the following as the most dominant features for predicting piezo behavior:

- V_i : The currently applied voltage.
- ΔV_i : The difference between the current and previous voltage steps.
- $\sum_{i=t-59}^t \alpha^{t-i} V_i$: A rolling exponential sum of the past 60 voltage steps.
- $\sum_{i=t-299}^t \alpha^{t-i} V_i$: A rolling exponential sum of the past 300 voltage steps.
- D_{i-10} : The piezo displacement lagged by 10 time steps.
- $\frac{1}{10} \sum_{i=t-9}^t D_i$: The rolling average of the piezo displacement with windows size 10.

These selected features will serve as the input to the subsequent machine learning models (neural networks, LSTMs, and KANs), enabling a focused and efficient learning process for predicting piezo hysteresis and creep.

4.3 Hyperparameter Optimization

To achieve optimal model performance, careful hyperparameter tuning is of essence. In this study, we employed distinct strategies for different models:

- **NN and LSTM:** The Optuna framework is used to automate the search for the best hyperparameter configurations. This approach facilitates efficient exploration of the hyperparameter space, leading to the identification of optimal settings for both models.
- **KAN:** Due to its novelty and lack of integration into common frameworks at the time of this study, the KAN’s hyperparameters are manually tuned based on recommendations from the associated GitHub repository [18].

This dual approach ensured a fair comparison between the NN and LSTM models, which benefited from automated optimization over 500 trials, and the KAN model, which relied on expert guidance for hyperparameter selection.

The specific hyperparameters considered and their optimal values which are used to train the final models are detailed in Table 2.

Table 1. Hyperparameter Search and Optimal Configuration

Model	Parameter	Search Space	Optimal Configuration
Dense	Depth	1-5 hidden layers	1 hidden layer
	Width	1-20 neurons per layer	10 neurons
	Optimizer	Adam, RMSprop, or SGD	Adam
	Learning Rate	1e-5 to 1e-1 (log)	1e-3
	Activation	Leaky ReLU (fixed)	
	Training Epochs		50
LSTM	Layers	1-5 LSTM layers	1 LSTM layer
	Hidden Size	4 or 64 features	29 features
	Optimizer	Adam, RMSprop, or SGD	Adam
	Learning Rate	1e-5 to 1e-1 (log)	1e-3
	Training Epochs		45

Table 2. Hyperparameter Search Spaces (explored over 500 trials) and optimized configurations for NN and LSTM Model

5 Evaluation

5.1 Model Performance

The performance of the four models is displayed in Table 3. It shows the error of piezo hysteresis and creep prediction as the Mean Absolute Error (MAE) of the deviation of the predicted and measured position in nanometers. The KAN model performs best with an MAE of 8.17 nm for hysteresis and 9.94 nm for creep. Notably, the linear regression model performs almost equally well, especially for hysteresis prediction. The vanilla NN, while capable of capturing nonlinear relationships, exhibits the highest error for both phenomena, its MAE being 3.79 nm and 7.28 nm higher than the KAN model for hysteresis and creep, respectively. With an error of 8.73 nm for hysteresis and 10.26 nm for creep, the LSTM model shows competitive performance.

Table 3. Mean Absolute Error (MAE) of Models for Hysteresis and Creep Prediction (in nm)

Model	Hysteresis MAE	Creep MAE
Linear Regression	8.20	10.0
Vanilla NN	11.96	17.22
LSTM	8.73	10.26
KAN	8.17	9.94

5.2 Hysteresis

Figure 11 shows the recorded and predicted hysteresis for a sawtooth function with increasing amplitude. The largest error for the vanilla neural network occurs at the inflection points of the applied voltage. The predicted position of the LSTM shows a moderate error throughout the movement, but it usually captures the hysteresis. for the KAN, a minimal error occurs during the rising part of the voltage curve. When evaluated

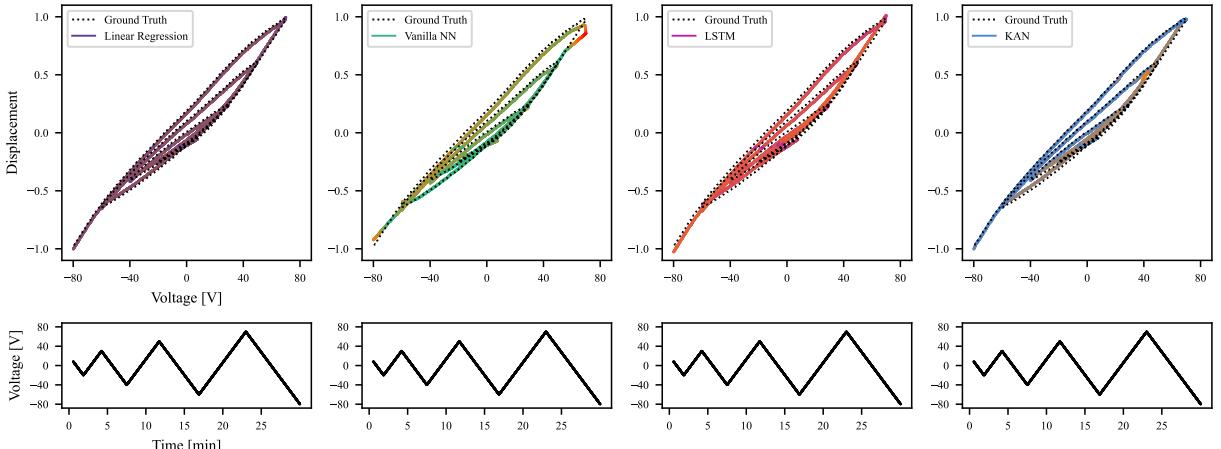


Figure 11. Recorded and predicted hysteresis for a sawtooth input with increasing amplitude. The vanilla neural network (NN) shows the highest error at the turning points. The LSTM model shows moderate but consistent error, while the KAN and linear regression models show minimal error, especially during the rising voltage phase.

on the data generated by the random walk, as shown in Figure 12, the LSTM again shows a small error over larger periods, while the predictions from the KAN and linear regression are near perfect for most of the input voltage. The NN shows a low prediction error overall however, during with some sections it has the highest errors of all the models.

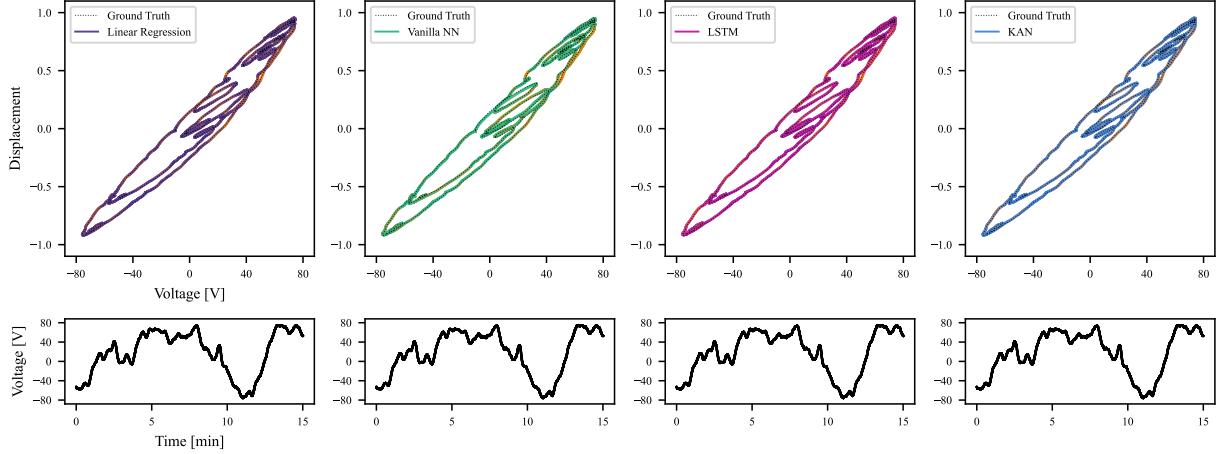


Figure 12. Recorded and predicted piezo displacement for a random walk voltage input. The LSTM model shows a small but persistent error over time. The KAN and linear regression models show near perfect agreement with the recorded data for most of the trajectory. The vanilla NN model shows sporadic spikes in error.

5.3 Creep

Figure 13 shows the model predictions along with the ground truth creep behavior exemplary for four of the fifteen recorded scenarios. All models capture the rate and amount of creep that occurs during the recording. In one case the NN introduces a error of more than 25 nm in the first minute of the time frame and is not able to recover from it. This results in a continuous error for the remaining duration of the recording. The LSTM shows a similar error in the beginning, but manages to correct it over time and is closer to the true position in the end than the NN. Linear regression and the KAN model show no such problem in this particular scenario. Another deviation occurs in the examples

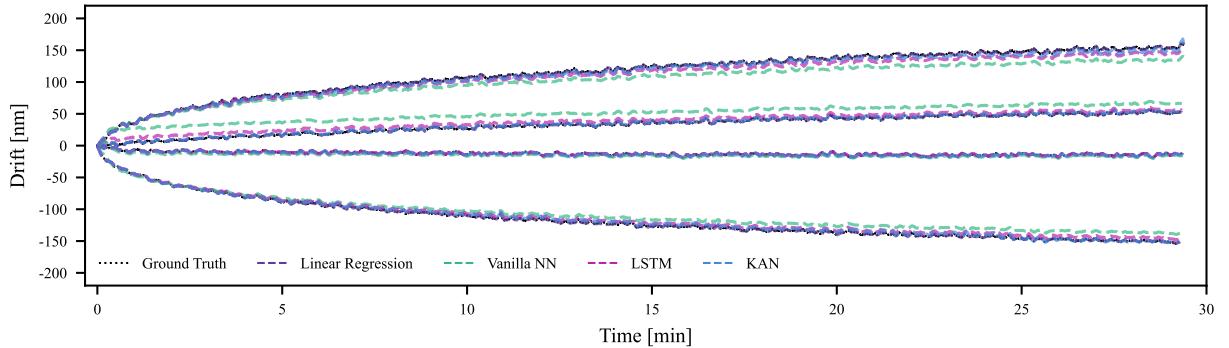


Figure 13. Recorded and predicted piezo creep for 4 different histories of applied voltages.

with the highest negative and highest positive drift of Fig. 13. The LSTM and especially the NN seem to have a tendency towards underestimating the amount of drift occurring.

They start with a low error prediction, but after around 10 minutes the predictions start to deviate from the ground truth. This continues until the end of the recording.

To further evaluate the long-term creep prediction capability of the models, the final position is averaged over the last 5 seconds of each 30-minute recording. Figure 14 shows the deviation of the predicted final position from the ground truth for all 15 recorded series. The error bars represent the quantified encoder noise (see section 4.1.1). The KAN and linear regression models perform consistently well, with deviations of less than 10 nm. The LSTM model shows mixed results, outperforming other models in some cases but showing larger deviations in others. The Vanilla NN model consistently shows the largest deviations, exceeding the encoder noise level four times.

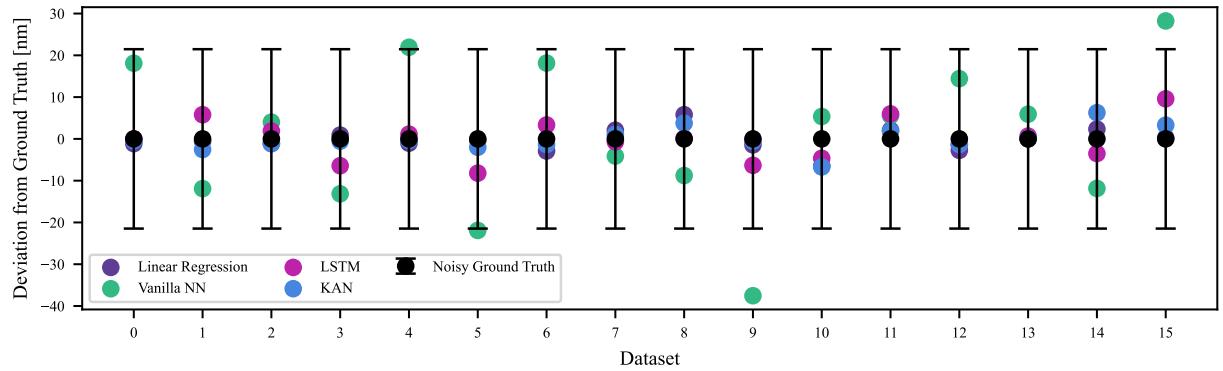


Figure 14. True and predicted position after 30 minutes of creep. Encoder readings underlay noise with a standard deviation of 20.79 nm.

6 Discussion of Model performance

The results presented in the previous section highlight the capabilities of different machine learning models in predicting the complex hysteresis and creep behavior of piezos. The KAN model consistently outperforms other approaches, demonstrating its ability to capture subtle nonlinearities and long-term dependencies in the piezo response. The strong performance of the linear regression model, especially for hysteresis prediction, suggests that a significant portion of the piezo behavior can be explained by a linear relationship of the features used, at least within certain operating regimes. The LSTM model, while promising, struggles with accumulating errors over time, possibly due to the challenges of modeling long-term dependencies in recurrent networks. The vanilla NN, despite its capacity for nonlinear modeling, exhibited the highest errors, possibly due to overfitting or difficulties in capturing the specific patterns of hysteresis and creep.

The strong performance of the KAN and linear regression models in modeling hysteresis and creep is particularly promising for the development of effective compensation strategies. The relative simplicity of these models compared to more complex neural networks facilitates the extraction and interpretation of their learned parameters.

In the case of KAN, the learned activation functions at the edges can be expressed as relatively simple mathematical functions of the input features. Similarly, the coefficients of the linear regression model directly represent the linear relationship between the input voltage features and the predicted piezo displacement.

This ability to express the learned models in a compact and interpretable form is crucial for their practical implementation. It enables the development of compensation algorithms that can be efficiently implemented on the micromanipulator's controller, allowing for real-time correction of hysteresis and creep effects. By integrating these compensation strategies directly into the control system, we can achieve more robust and precise positioning of the probe tips, ultimately increasing the reliability and accuracy of nanoprobe operations.

7 Conclusion

The present study explores the potential of machine learning (ML) for modeling and predicting the complex hysteresis and creep behavior of piezo actuators, which are critical components in nanoprobe systems for semiconductor failure analysis. The study evaluated the performance of several ML models, including linear regression, vanilla neural networks, LSTMs, and the novel Kolmogorov-Arnold network (KAN). The promising results obtained with the KAN model in capturing both hysteresis and creep warrant further investigation of its capabilities and potential applications, highlighting possible improvements for the accuracy and reliability of piezo-driven systems.

The results of this study demonstrate the potential of ML models in the field of nanoprobe and semiconductor failure analysis. The development of accurate and efficient models for predicting piezo behavior can lead to the implementation of real-time compensation strategies that enable more precise and stable positioning of probe tips. This, in turn, can improve the quality and efficiency of semiconductor testing, ultimately contributing to advances in electronics manufacturing and nanotechnology research.

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