

A supervised machine learning approach to a predictive model of nanoscale friction

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Abstract

Modelling of nanoscale friction presents a long-lasting challenge. In fact, while there are several generalised models that provide good results for macro- and micro-scale friction, due to the complex concurrent physicochemical interactions in nanoscale contacts, when modelling nanoscale friction there is a clear lack of reliable predicting tools. The modelling methodology proposed in this work is based on the recently performed multidimensional experimental measurements of thin-films' nanoscale friction, where the concurrent effects of several process parameters are considered. Due to the stochastic nature of the considered phenomena, conventional regression methods yield poor predictive performances. A machine learning (ML) numerical paradigm is hence proposed. Via a comparative study it is hence shown that, while the best typical regression models result in coefficients of determination (R^2) of the order of 0.3, the predictive performances of the used ML models, depending on the considered sample, yield R^2 in the range from 0.54 to 0.9. The developed models provide also new insights into the functional dependence of the variable process parameters, but also sound basis for future extensions of existing friction models to the nanometric range.

Nanoscale friction, mathematical modelling, machine learning, predictive model

1. Introduction

Due to complex physicochemical interactions in nanoscale contacts, nanoscale frictional behaviour is still matter of intense studies. Empirical insights, obtained via thorough experimental procedures [1], are used in this work as the foundation for the development of a predictive nanoscale friction model. The experimental procedure, involving scanning probe microscopy in the lateral force microscopy mode, includes measurements of nanoscale friction force F_f vs. the variable process parameters (normal force F_N , sliding velocity v and temperature \mathcal{G}) on thin-film samples synthesized via atomic layer (ALD - Al_2O_3 and TiO_2) and pulsed laser deposition (PLD - Al, MoS_2 and stainless steel X39CrMo17-1) [1]. Data collected on the 50 experimental measurement points, defined by employing centroidal Voronoi tessellations (CVT), are hence used as the main dataset for the development of the models. Each models' predictive performance is tested by employing the same experimental technique on a separate set of 15 points defined randomly via the Monte Carlo (MC) method [2]. Modelling by conventional methods for regression analysis, e.g. polynomial fitting, response surface methodology etc., yields poor results. Machine learning (ML) is thus proposed and the obtained results are thoroughly assessed.

2. Used methodology

Methods used in this work comprise various ML algorithms. ML algorithms for regression problems deliver a so-called black-box solution that provides predictive results. These methods are used for obtaining important insights into the analysed variable space, providing the basis for further studies. The ML algorithms used in this work, according to the proposed methodology shown in Fig. 1, are additive regression, stacking and bagging classifiers, lazy algorithms, multi-layer perceptron (MLP), support vector regression (SVR), decision trees and random forest (RF) ensembles [3]. All of them are used to develop nanoscale friction models for each considered sample material

via the following steps: data preparation (normalization, standardization), training the algorithms on experimental datasets and optimizing each of their hyper-parameters. The training is performed here on the complete CVT-based datasets for each material separately, as well as, by employing binary encoding for a material class, on the combined (pooled) dataset of all materials subjected to a 10-fold cross-validation. The metrics used for evaluating the developed models are mean absolute errors (MAE), root-mean square errors (RMSE) and coefficients of determination R^2 [4].

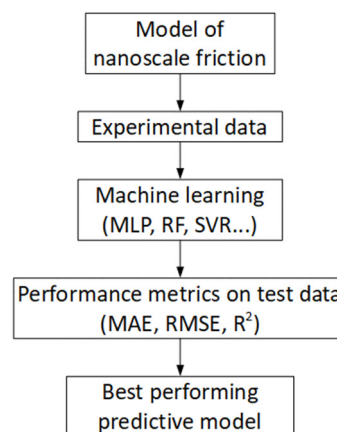


Figure 1. Proposed methodology for the development of a predictive model of nanoscale friction.

3. Testing dataset

Separate experimental measurements, on an un-seen testing dataset whose results are aimed at a best possible prediction via the usage of the developed models, are performed next. It is worth noting that these measurements are performed on samples that are not dried prior to the measurements – yielding, hence, not only realistic conditions but also providing a more difficult predictive challenge for the used advanced numerical

models. Each model's predictive performance is hence scrutinized on the predictions of the friction forces F_f on this testing dataset for changing input variables. Fig. 2 depicts a colour-coded representation of the obtained F_f values for Al_2O_3 (a sample of ALD-synthesized thin-film) and for MoS_2 (PLD-synthesized thin-film – data for all the considered thin-films is given in [5]) vs. the variable parameters. The total applied normal load is constituted here by the sum of the exerted normal force (F_N) and the contribution of adhesion (F_A). Experimental measurements show clearly the stochastic effects of the variable process parameters on F_f , but with similarities to the results attained on CVT-based measurements datasets [1].

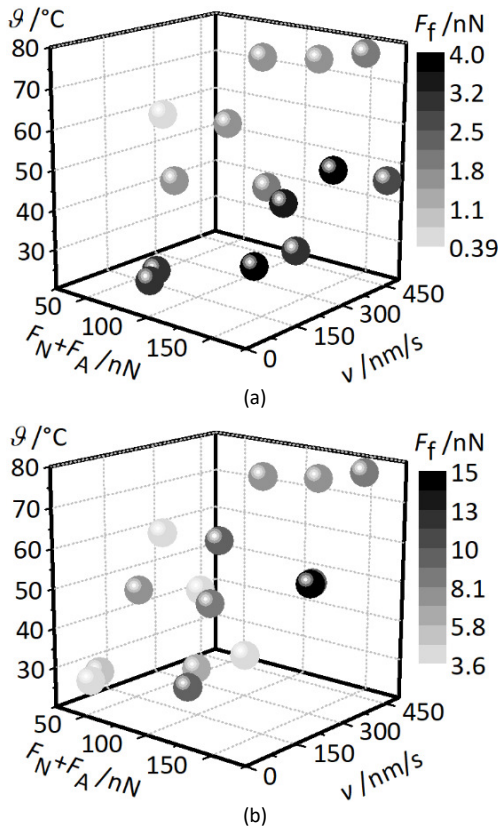


Figure 2. Colour-coded distribution of experimentally determined F_f values for the test dataset for Al_2O_3 (a), and MoS_2 (b).

4. Results and discussion

All ML models allow attaining far better predictive performances (higher R^2) than the conventional regression methods. The ML models developed by training the algorithms on a pooled (combined) dataset show even better predictive performances. The obtained predictive performances on the MC-based test datasets for each developed ML model are shown, for the two sample thin-film materials, in Fig. 3, where the achieved R^2 values for each algorithm, for the best-performing models, are given in parenthesis. Fig. 3 also denotes the uncertainty levels in three shades of grey presenting, respectively, $\pm 1\sigma$ (darkest shade), $\pm 2\sigma$ and $\pm 3\sigma$ (lightest shade), variance of data [4]. It can thus be seen that, even though the MLP algorithm allows attaining high R^2 values, it is quite far away from the experimental data. On the other hand, the RF and SVR predictions follow the data much better. The test data predictions for MoS_2 (Fig. 3b) are much better than that for Al_2O_3 , with the SVR algorithm capturing in this case 90% of the F_f variance. The deviations of the attained predictive performances of each model are caused here by the combined effects of the inherent models' properties, i.e., by the smoothness of the solutions (hyperplanes), by the normality

characteristics of the used experimental datasets, and finally, by the intrinsic stochastic nature of nanoscale friction.

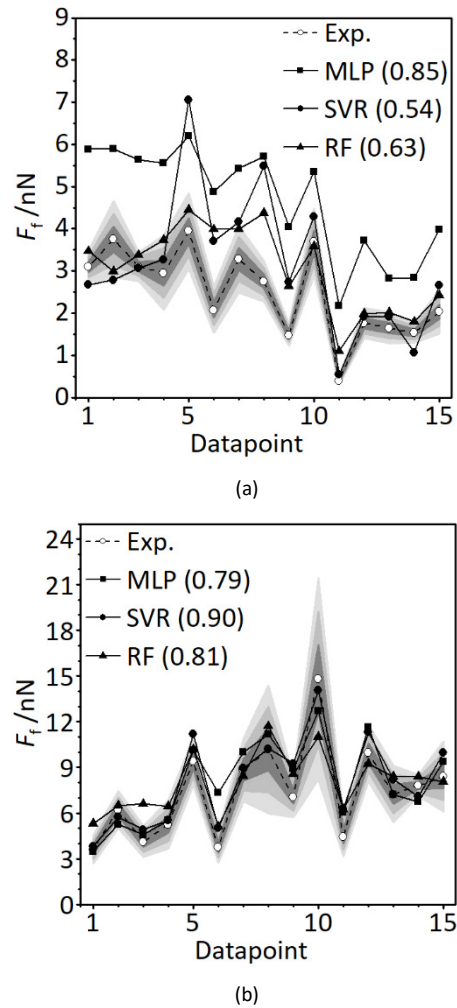


Figure 3. Predictive performances of the considered ML models on the MC test dataset for Al_2O_3 (a), and MoS_2 (b).

5. Conclusions and outlook

The analysis of the nanometric frictional behaviour, performed by using the black-box ML models, proves that it is possible to provide effective predictions of the influence of the multiple process parameter on the value of the friction force with satisfactory levels of accuracy, i.e., with the R^2 values ranging from 0.54, for the SVR algorithm on an Al_2O_3 sample, to 0.9, for the SVR prediction on an MoS_2 sample.

Further numerical analyses, performed by employing novel artificial intelligence-based methods such as genetic programming, will be used in the next phases of the work to fully characterize the functional dependencies of nanoscale friction.

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