Supporting Information

How Machine Learning Will Revolutionize Electrochemical Sciences

Aashutosh Mistry,[*,†] Alejandro A. Franco,[*,‡] Samuel J. Cooper,[*,⊥] Scott A. Roberts,[*,#] and Venkatasubramanian Viswanathan[*,@]

†*Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, United States*

‡*Laboratorie de Réactivité et Chimie des Solides (LRCS), UMR CNRS 7314, Université de Picardie Jules Verne, Hub de I'Energie, 15 rue Baudelocque, 80039 Amiens Cedex, France*

¶*Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, Hub de l'Energie, 15 rue Baudelocque, 80039 Amiens Cedex, France*

§*ALISTORE-European Research Institute, FR CNRS 3104, Hub de l'Energie, 15 rue Baudelocque, 80039 Amiens Cedex, France*

‖*Institut Universitaire de France, 103 Boulevard Saint Michel, 75005 Paris, France*

⊥*Dyson School of Design Engineering, Imperial College London, London SW7 2DB, United Kingdom*

#*Engineering Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico 87185, United States*

@*Department of Mechanical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, United States*

E-mail: amistry@anl.gov; alejandro.franco@u-picardie.fr; samuel.cooper@imperial.ac.uk; sarober@sandia.gov; venkvis@cmu.edu

Model Parameters and Data Accuracy

As mentioned in the manuscript, data-driven ML models fundamentally approximate the trends underlying the dataset. Often data contains variability (*e.g.*, noise in measurements) and instead of each datapoint considered as an accurate representation of system behavior, the datapoints are treated collectively to infer the mean trends. In other words, the choice of ML model is related to the trends a researcher wishes to infer. This process is guided by researcher's intuition, experience and quantitative descriptors of model fidelity. The model selection process can be broken down into two aspects:

- Type of approximation, for example, neural networks *vs.* gaussian process regression;
- Parameters in the approximation, for example, how many hidden layers and how many neurons in each hidden layer in a neural network approximation.

The first aspect is largely governed by intuition and experience. In the context of physics-based ML, the physics provides additional information such as continuity and differentiability of the approximation - in the $D = D(T)$ example in Fig 2, the slope ${}^{\mathrm{d}\log D}/_{\mathrm{d}(1/T)}$ is related to activation energy and has a physical meaning.

The second aspect of identifying parameters has relatively straightforward quantitative guidelines, and is referred to as Bias-Variance Trade-off or Cross-validation.[1] The idea is to split the dataset into (at least) two subsets - one for training and another for testing. Once the model type is fixed (say neural network), number of model parameters is assumed, the model is subsequently trained for these many parameters and the predictions of the trained model are compared against the testing set. This process is repeated for multiple parameter counts to construct (i) training error vs. # parameters and (ii) testing error vs. # parameters plots. The training error improves with parameter counts and usually exhibits a monotonic dependence. Alternatively, the test error improves initially, plateaus and starts diverging at higher degrees of parameterization. Accordingly, the optimal approximation is the one with the smallest train and test error. Some recent studies[2] demonstrate that the test error

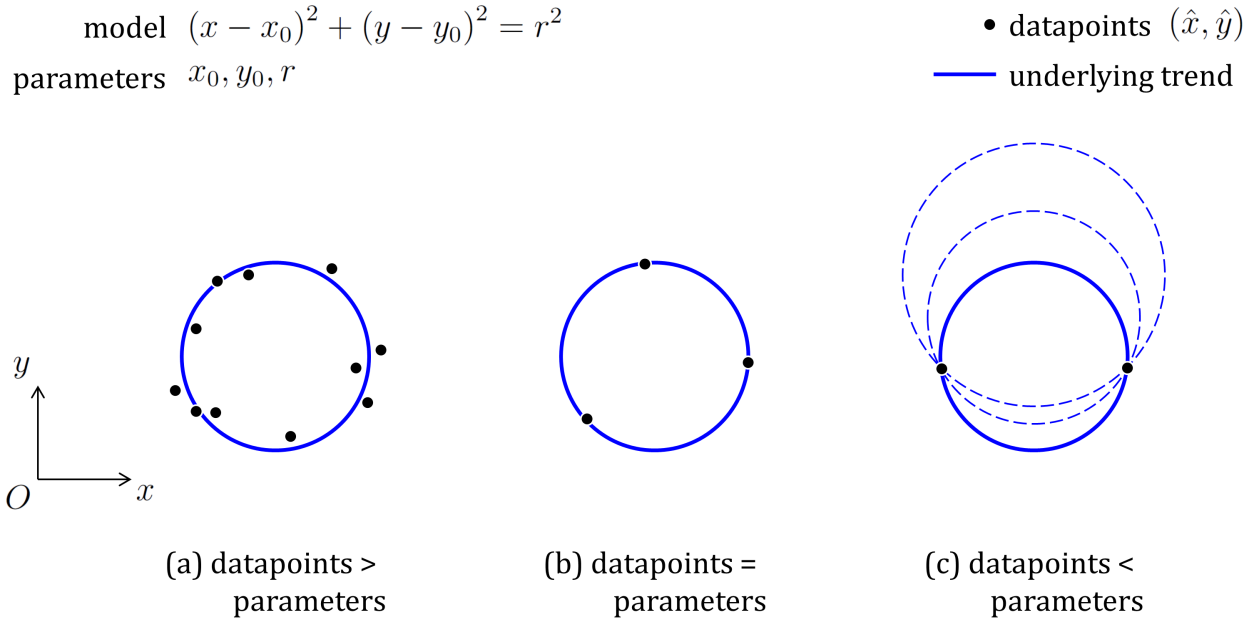

Figure S1: For a given dataset, three approximations are possible based on the degree of parameterization. (a) Regression deals with more datapoints than the parameters, while (b), (c) interpolation has as many parameters or more. Implicitly, these categories relate to the reliability of the datasets.

has a more involved relationship with the degree of parameterization. Instead of a diverging test error at higher parameterization, it increases and then decreases again (referred to as the *double descent* phenomenon) to provide superior predictions. Thus, one should explore a sufficient range of parameterization to identify an optimal approximation. If the optimal approximation chosen based on such error landscapes exhibits large errors, one can modify other details of the approximation. For the neural network example, one can try different activation functions or the input features and output labels may be preprocessed (sometimes referred to feature engineering) to improve predictability. Each such design choice will lead to a new set of error landscapes to help identify corresponding optimal approximation.

An upper bound on the degree of parameterization is set by the datapoints in the training set. For an N datapoints set (N points for every input feature), at most N parameters can be uniquely identified. One has to provide additional information to identify extra parameters. To pictorially illustrate this, let us consider identifying a circle $(x-x_0)^2+(y-y_0)^2=r^2$ from given dataset $(\hat{x},\hat{y})$.

This model has three parameters (x_0, y_0, r), and require three linearly independent datapoints to uniquely identify these parameters (Fig S1(b)). If less datapoints are available, additional information is needed to find a unique parameter set. For example, multiple circles, *i.e.*, different (x_0, y_0, r), pass through two datapoints. Additional information that identifies a relationship among parameters is needed to find a unique set. In this example (Fig S1(c)) a circle passing through the two points and having the smallest radius, r, is unique. In the other extreme, when too many datapoints are avialable (Fig S1(a)), a unique parameter set can be identified in the least squares sense. Let (x_i, y_i) be the underlying trend at the datapoint $(\hat{x}_i, \hat{y}_i)$. A unique parameter set exists that minimizes the error

$$E = \sum_i (\hat{x}_i - x_0)^2 + (\hat{y}_i - y_0)^2 - r^2$$

Classically, Fig S1(a) is a regression problem, while Fig S1(b-c) are interpolations.[3,4] Fundamentally, the choice of regression vs. interpolation relates to the reliability of the data. If the datapoints contain variability, the underlying trends should be identified using regression; while if the datapoints represent true system response, interpolation is a logical approach. Most non-scientific ML implementations build on field data and accordingly perform regression. However, the physics-based ML deals with high confidence datasets such as generated from a physics-based simulation and allows us to explore interpolation (e.g., Fig 5). End of the day, one must treat experimentally generated data (*e.g.*, cell performance), physics-based stochastic calculations (*e.g.*, monte carlo) and physics-based deterministic simulations (*e.g.*, porous electrode theory) as different datasets with intrinsically different reliability levels.

ML Applications - an Extended List

Besides good Machine Learning (ML) textbooks,[1,5–8] the following list provides references to different ML applications. Given the nascent state of ML applied to scientific fields, not all examples are from the electrochemical systems.[9,10] We also include interesting examples

from other fields that have potential application to the electrochemical systems.

Structure - property mappings [11–41]

Mesostructure Generation [42–52]

Property - performance mappings [53–64]

Control and Automation [65–72]

Miscellaneous [61,73–91]

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