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Developing a Physics-Informed Neural Network to Predict Soil Reaction Fronts

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Reaction fronts in the soil profile have been simulated by numerous physics-based models (PBMs), which are usually hard to parameterize. Unlike PBM, the neural network (NN) model yields superior predictive capabilities while requiring significantly less domain knowledge. The most common criticism for the data-driven NN model is the inability of humans to understand the process and the associated physics laws.

In this work, we integrated a PBM with a NN to simulate the depth profile of feldspar dissolution in soils. Specifically, we explored this hybrid neural network (HNN) to see if it could predict reaction fronts as a function of important variables known from domain knowledge: temperature (T), precipitation (P), soil residence time (t), erosion rate (E), and quartz content (Q) and albitic feldspar content of the feldspar (A) in the parent material. We evaluated the mean square error (MSE) for 63 HNNs, each using a different combination of soil profiles and environmental variables. The HNNs were often better at predicting the slope than the depth of the reaction front, which is constrained by the original PBM. The most and least effective variables in predicting the soil profile, according to HNN results, were t and P.

We also developed a tool to identify cases of local rather than global convergence. Specifically, we compared the MSE of HNN to that of the corresponding PBM as well as HNNs that used a subset of the environmental variables as predictor variables. Our preliminary results suggested that HNNs trained to four or five soil profiles and using a subset of t, T, Q, E, and A as predictor variables were globally converged, as measured by lower MSEs than the PBM. To achieve an MSE within 1% of the corresponding PBM, at least two variables were required to train an HNN. The approach shows promise for future efforts but should be applied to larger sets of soil profile data and PBMs that predict both the depth and slope of reaction fronts.