How AI Predicts the Untrained and Unseen

-A Deep Learning - Physics - Observation Hybrid Approach for Future Water Cycle Under Extreme Conditions

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Focus Area: Model predictability improvements (Primary); Data optimization (secondary); Data complexity insights (secondary)

The Challenge

If we believe that a future under extreme conditions will look very differently from today, we can likely agree that ML/AI models trained on past and present datasets will not be adequate to make reliable predictions into the future. This is true for water cycling, as well as biogeochemistry and other Earth system components and behaviors. Additionally, ML/AI models are inherently non-physical. Despite the flourishing success of ML/AI in many applications, such as computer vision, natural language process, and gaming, even the most sophisticated AI models don't understand the very basic physical laws. Therefore, a natural question is: Can we trust ML/AI based predictions of Earth system behaviors that are fundamentally driven by physical laws?

So, are physics models with meticulous process representation a better choice? Not exactly. Physical models, when firmly rooted in first principles, work great at predicting behaviors of systems with a well-defined set of boundary conditions and variables. However, as a complex system, the number of parameters and the degree of complexity and dynamics in processes, coupling, and scale dependent emergent behaviors make the Earth system behaviors very challenging to predict with physical models composed of deterministic laws. In addition, due to the lack of fundamental understandings, physical models often implement empirical correlations derived from observations with biases from locality of data generation. Because correlation is not necessarily causation or comply with first principles, scaling of model predictions beyond locality is often invalid.

Beyond the limitation of models, physics or AI, our knowledge of the Earth system is limited by the lack of observational technologies and resources. Insufficient data density, dimensionality and diversity only offer a sliced (or projected) view of the Earth system, e.g. Plato's Cave analogy, limiting our capability to better understand and represent fundamental processes in models.

The Solution: A hybrid DL – physics - observation roadmap

Despite being non-physical, AI models embrace complexity. Deep learning (DL) models thrive by exploring the differentiability and inter-dependency in an often very large parameter space. An extreme example is the latest GPT3 (Generative Pre-trained Transformer) model with 175 Billion parameters. This type of complex DL models appears to resemble the level of complexity in Earth systems, and has been proven to have significant predictive power, albeit only for non-physical applications such as natural language processing.

As stated, AI models trained on past and present datasets cannot predict a different future under extreme conditions. Adapting AI models to radically improve Earth system predictability with trustworthiness and physics representation can be realized by the hybridization between AI and physics models, and their critical dependence on new observational platforms and technologies for measuring new parameters, discovering new physics, and establishing new boundary conditions non-existent in the past and the present.

A few key elements of such an approach is described below:

DOI: https://doi.org/10.2172/1769716
DOE BER, AI4ESP 2021 #AI4ESP1146 (https://www.ai4esp.org)

1. **Extreme scenario representation in AI training datasets**: AI models for the prediction of extreme events need to be adequately trained with datasets representing extreme conditions. In other words, AI models cannot predict a probability distribution not seen during training. Yet, extreme events and associated datasets are sparse by definition. A potential solution is to jointly use manipulative experiments with physics models and generative AI models, such as the Generative Adversarial Nets (GANs). By optimizing a Minimax Value Function toward a Nash Equilibrium between a Discriminator and a Generator Net in a lock-step process, GANs can be used to generate a massive number of realistic extreme event datasets after properly trained. For our application in water cycling, manipulative experiments are designed to simulate future extreme conditions. These experiments are used to build, improve and validate new physics models for extreme events. The physical models can then be used to generate an ensemble of true training datasets as inputs to the discriminator in GANs, which can be used to generate a large number of extreme datasets after being properly trained. Such datasets can be used in a variety of other ML/AI applications under future extreme scenarios.
2. **AI-aware observational strategy**: In additional to improving physics models, the data collection strategy should keep their applications in AI models in mind, and this often ties with the AI algorithm of choice. For example, the Transformer Net offers an exciting opportunity to assess existing Earth datasets and to guide new data collection efforts. Specifically, the multi-headed attention functionality in Transformer Net offers a mechanism to capture the inter-dependency among different data types, such as evapotranspiration and radiation, and the "attention" one type of data should pay to others during the training process. This attention mechanism can be used to guide data collection efforts that best improve correlations between datasets for better algorithm training and causal discovery.
3. **AI algorithm selection that best fits data**: Earth system observational datasets span a large range from sample based, to point sensors to satellite imageries, and include datasets with large spatial coverage as well as those with long time series. Selection of AI algorithms needs to consider their fitness and computational efficiency for the data types, and that such algorithms are evolving rapidly. For example, Transformer Nets are superior in computational efficiency in handling long time series/or relational datasets when compared to typically used recurrent neuron networks, such as LSTM (Long Short Term Memory) and GRU (Gated Recurrent Unit). This is because Transformer Net can fully explore the parallelization power in GPU by computing attentions between all datapoints concurrently, instead of going through the recurrent steps one by one during gradient decent training process.
4. **Hybridization of physics into AI algorithms**: The training of AI model is a process of optimizing weights and biases in a massive parameter space with no physical meanings. The approach described above is a de-coupled approach where physical models are only used to generate realistic inputs to train AI models, with the hope that if the data AI algorithm sees make physical sense, then the predictions are not violating physical laws. This seems to make sense, but is difficult to validate. Direct coupling between AI and physics models might be possible and, if realized, could significantly improve the trustworthiness of the predictions made by AI models. One potential mechanism is to build a physics law based residual connection in the feedforward link between hidden layers of a deep neuron network, so the feature prediction is constrained by physics. The residual connection method was introduced to resolve optimization deterioration issue as the neuron network gets very deep. A DL algorithm for complex Earth system likely gets very deep, and the introduction of a physics law based residual connection may not only stabilize the network, but also introduce "physics-ness" into a non-physical process. Take surface temperature and effects on ET as an example. By applying a residual connection that takes second order spatial derivative to surface temperature and feedforward into the next layer convoluted with a kernel to extract its temporal gradient could introduce physics constraints to the prediction of temperature evolution, and subsequently ET dynamics, because its compliance with the heat equation.

An Example: Future Water Cycling Under Extreme Conditions

The approach described above is a generic framework and it could be challenging to grasp without describing a specific application. An example is given here that focuses on accurate ET prediction at watershed scales under future extreme conditions. This is done by integrating multi-scale measurements across lab and field, mechanistic ET and other physics models, as well as the joint use of multiple AI algorithms.

Following the framework described above, the solution starts with constructing and benchmarking ET models, such as Penman-Monteith, utilizing experimental data collected on platforms mimicking future extreme conditions, e.g., severe droughts. The model construction and benchmarking process also evaluates parameter sensitivity, uncertainty, and critical new parameters that need to be measured, which guide new sensing development needs. The ET model also links with other physical models, such as Richard's equation that drives soil moisture dynamics which impact soil surface resistance, a parameter important for ET. New physical models benchmarked by the manipulative experiments will then be used to generate an ensemble of simulations which feed into generative AI models, such as GANS, for training. Once trained, GANs can produce a massive number of ET scenarios under variable conditions (e.g., topography, radiation, vegetation cover), which resemble target field conditions. Scaling of the ET models into the future relies on the use of additional AI algorithms that handle time series and relational datasets, such as the Transformer Nets described above. Joint use of GANs and Transformer Nets allows the scaling from one grid cell (e.g., 1 km^2) to a much larger domain (e.g., 30 x 30 km^2), and from the present to the future by jointly using both spatially extensive remote sensing data (but lacks temporal resolution), temporally extensive plot scale sensor data (but lacks spatial coverage), and everything in between. Surface temperature evolution is a key process for ET dynamics, and the heat equation could serve as a residue connection between the hidden layers of the various neuron networks to ensure that temperature evolution trajectory follows physical laws. It is likely we will discover data deficiency during this process which will be used to guide new experiments, new sensor developments, and new data collection campaigns.

The Ten-year Outlook

Of the four key elements in AI, data are of the most pressing need for earth system predictability. The rapid development of the convolutional neuron networks would not have been possible without the construction of a few large, high quality datasets, such as the ImageNet. AI has come a long way since ImageNet and there is an unprecedented opportunity to optimize data collection efforts guided by AI models in the next ten years. This includes not only the collection of more data, but also technology innovation to enable the collection of more types and dimensions of data to overcome the Plato's cave Conundrum in Earth observation.

We have witnessed the rapid acceleration of AI in the last few years, e.g., the invention of GANs and Transformer Nets, and the broadening of their applications, including in Earth sciences. We can expect such a trend to continue to accelerate. Ten years is a long time in AI age and the acceleration toward artificial general intelligence (AGI) seems inevitable. The recent development of GPT3 and its trial release (as an API) give us a glimpse of its possibilities and the potential applications in Earth systems. Therefore, it is critical to monitor and properly adopt the new developments in AI for Earth system applications.

Earth science and other scientific disciplines face the challenge of how to incorporate physics laws, which govern the behaviors of the Earth system, into AI models to improve its fidelity and trustworthiness. Developing a generalizable framework to couple physics and AI models seems a necessity, but a long process. The development toward AGI offers new opportunities that need to be captured. A specific mid-range example could be a scientific version of GPT3 for massive meta-analysis applications to discover new physics insights which can be reinforced in the algorithms for applications such as improving Earth system predictability.