

- Link to the comparison of 8 surrogates across the dimensions defined below:  
<https://github.com/radical-group/esraa/blob/master/Weekly%20Summaries/Week%2012.pdf>

### Changes:

- Updated the classification to ensure that I 1)use clearly defined terms and 2)use terms consistently
- Removed performance dimension since meaningful quantification of performance improvement is surrogate-specific.

### Surrogates Classification:

- **Functionality Dimension:** concerned with the functionality of the surrogate and the link between ML and HPC:

\* *Link between ML and HPC:* HPCforML uses HPC to execute and enhance ML performance, or uses HPC simulations to train ML algorithms, which are then used to understand experimental data or simulations. MLforHPC uses ML to enhance HPC applications and systems [10].

\* *Functionality:* Smart surrogates can fulfill different functionalities including 1) Use HPC simulations to train surrogates. This can be done by engaging supercomputing resources to take advantage of high-dimensional training data produced from simulations and/or experimental data to train a neural network to predict an event of interest (For example, predict disruptive instabilities in controlled fusion plasmas) [23], 2) replace an internal simulation component (for example, learn an accurate and transferable potential for organic molecules) [24], 3) to guide computations (for example, choose the optimal training data) [26], and 4)to extract patterns.

Note: Surrogates that require the use of summary statistics cannot serve as universal approximators . Thus, having the ability to learn the underlying distributions of data and emulate the observable without imposing the choice of summary statistics, as in the traditional approach to emulators, is valuable.

- **Problem Dimension:** concerned with the algorithmic area and the dimensionality of the problems.

\* *Algorithmic area:* The scientific problem the surrogate is investigating. For example: partial differential equations, particle dynamics.

- **Algorithmic dimension:** concerned with the machine learning model used and the resulting architecture and its properties.

\* *Machine learning model:* most work to date in building surrogates uses random forests[4], Gaussian Processes[5], CNN[14], FCN[20], RNN[20], or other machine learning models [6,7]. Non- Neural Network models have limited ability to model high-

dimensional inputs/outputs. Dimensionality reduction techniques can enable higher dimensional inputs/outputs but the improvement is limited [21,22]. Thus, Neural Network models are more suitable for processing natural n-dimensional signals. However, most existing deep active learning methods are concerned with classification tasks while Neural surrogates are generally concerned with regression tasks.

\* Machine Learning Architecture: Neural surrogate can use different architectures to handle different tasks. Most neural surrogates have their own unique architecture. Recurrent neural networks (RNNs) powerfully handle sequential data by maintaining information in an internal state that is passed between successive time steps, in addition to taking into account new input data at every time step. Meanwhile, convolutional neural networks (CNNs) can learn salient, low-dimensional representations from high-dimensional data by successively applying convolutional and downsampling operations. Some neural surrogates use already existing architecture while others use new architectures.

Note: finding the “correct” architecture is instrumental in the successful learning of surrogate models. For example, CNN priors inherently rely on their architectures, one has to find an architecture that gives the suitable prior of a given problem. However, required optimal architecture is likely to change when training data changes. Therefore, it is important to have a variable architecture that can adjust with associated uncertainty

\* Variability of the architecture: Most surrogates used in scientific workflow use a fixed architecture [4-7]. However, a recent paper [14] successfully used NAS (Neural Architecture Search) in order to infer the architecture of the CNN-based neural surrogate. Further work needs to be done to use NAS with other NN models.

- **Data dimension**: is a sub-dimension of the algorithmic dimension. Concerned with the generation, labeling and selection of the data used to train the ML model.

\* Data set generation and labeling: in supervised (sequential) learning, the labeled data set is given beforehand and learning is performed afterwards (offline)[4]. In concurrent machine learning, the data set is generated and labeled as model training proceeds (Online) [8]. In active learning, we are given the unlabeled data, and we decide which ones should be labeled during the training process[9].

\* Data selection method: Most surrogates models require human intervention for the selection and adjustment of training data [4-7]. However, an active approach to surrogates learning that enables automatic training data selection has emerged in GP surrogates[15].

\* Data Volume: Since the training data generation typically involves numerical solutions of the underlying micro-scale model, a process that is often quite expensive, learning an efficient surrogate is a small data problem. Datasets vary in size from of a few hundred[18] or a few thousand[16,17,19] individual simulations. The dataset that one

uses to construct the model should be a good representation of all the practical situations that the model is intended for.

\* Data span: training and the testing examples could be drawn uniformly across all experimental runs (thus requiring low generalizability). On the other hand, training and testing data could be drawn from slightly different distributions (for example, using data from one reactor to simulate the performance of another reactor) [24].

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