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Neural network approach for robust and fast calculation of physical processes in numerical environmental models: Compound parameterization with a quality control of larger errors☆,☆☆

Vladimir M. Krasnopolsky[a,b,*], Michael S. Fox-Rabinovitz[b], Hendrik L. Tolman[c], Alexei A. Belochitski[b]

[a] *Science Applications International Corporation at Environmental Modeling Center, National Centers for Environmental Prediction, National Oceanic and Atmospheric Administration, MD, USA*
[b] *Earth System Science Interdisciplinary Center, University of Maryland, MD, USA*
[c] *Environmental Modeling Center, National Centers for Environmental Prediction, National Oceanic and Atmospheric Administration, MD, USA*

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Abstract

Development of neural network (NN) emulations for fast calculations of physical processes in numerical climate and weather prediction models depends significantly on our ability to generate a representative training set. Owing to the high dimensionality of the NN input vector which is of the order of several hundreds or more, it is rather difficult to cover the entire domain, especially its "far corners" associated with rare events, even when we use model simulated data for the NN training. Moreover the domain may evolve (e.g., due to climate change). In this situation the emulating NN may be forced to extrapolate beyond its generalization ability and may lead to larger errors in NN outputs. A new technique, a *compound parameterization*, has been developed to address this problem and to make the NN emulation approach more suitable for long-term climate prediction and climate change projections and other numerical modeling applications. Two different designs of the compound parameterization are presented and discussed.

Keywords: Neural networks; Numerical modeling; Climate; Weather; Waves; Data assimilation

1. Introduction

This paper describes an interdisciplinary study. This study follows upon our previous works presented in the previous papers of the authors (e.g., Krasnopolsky, Chalikov, and Tolman (2002) and Krasnopolsky, Fox-Rabinovitz, and Chalikov (2005)). In these works we developed a new approach, introducing nonlinear statistical learning techniques (NNs) into tremendously complex and time consuming numerical models, describing one of the most complex, multidimensional, and essentially nonlinear systems (climate/weather system) known to the modern science. This new approach introduces fast and accurate NN emulations of time consuming original model components into numerical climate/weather models. As a result, the model computational performance improves significantly without a detriment to the quality of model predictions. This applied research (and the current study) has a clearly formulated practical goal: to improve computational performance of operational weather prediction and climate simulation models by using accurate, fast, and robust NN emulations substituting the time consuming original components of the models.

1.1. Climate models and model physics

One of the main problems of development and implementation of high-quality high-resolution environmental models is the complexity of physical (chemical and biological) processes

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* Tel.: +1 301 763 8000; fax: +1 301 763 8545.
E-mail address: vladimir.krasnopolsky@noaa.gov (V.M. Krasnopolsky).

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involved. For example, for the state-of-the-art climate model, the National Center for Atmospheric Research (NCAR) Community Atmospheric Model (CAM) (see the special issue on the National Center for Atmospheric Research Community Climate Model in the *Journal of Climate*, 11 (6) 1998, for the description of the model), calculation of a model physics package takes about 70% of the total model computations. For this and other numerical models neural network (NN) techniques have been developed (Krasnopolsky et al., 2002, 2005; Tolman, Krasnopolsky, & Chalikov, 2005; Krasnopolsky & Fox-Rabinovitz, 2006; Krasnopolsky, 2007) for speeding up the calculations of model physics (i.e., deterministic or first principle components of atmospheric and oceanic numerical models describing physical processes) up to *two to five orders of magnitude*. The speed-up is achieved through the development of NN emulations of model physics.

Tremendous complexity, multidimensionality, and nonlinearity of the climate/weather system and numerical models describing this system lead to complexity and multidimensionality of our NN emulations and data sets that are used for their development and validation. Also, the validation procedure for developed NN emulations becomes more complicated because, after their development, they are supposed to work in a complex and essentially nonlinear numerical model. The development of NN emulations of model physics depends significantly on our ability to generate a representative training set to avoid using NNs for extrapolation beyond the domain covered by the training set. Owing to the high dimensionality of the input domain (i.e., dimensionality of the NN input vector) which is of the order of several hundreds or more, it is difficult if not impossible to cover the entire domain, especially its “far corners” associated with rare or extreme events, even when we use model simulated data for the NN training. Also, the domain may change with time as in the case of climate change. In such situations the emulating NN may be forced to extrapolate beyond its generalization ability which may lead to larger errors in NN outputs and, as a result, to errors in the numerical models in which they are used.

1.2. NN emulations of model physics

We have developed NN emulations of major components of climate model physics (Krasnopolsky et al., 2005; Krasnopolsky & Fox-Rabinovitz, 2006; Krasnopolsky, 2007) for the widely recognized and used NCAR CAM. Specifically, we developed the NN emulations of the NCAR CAM long wave radiation (LWR) and short wave radiation (SWR) parameterizations which are the most time consuming components of model physics describing the propagation of electromagnetic radiation in the Earth’s atmosphere. Both original (i.e. used in the current version of NCAR CAM) LWR and SWR parameterizations are physically based process models. They may be considered mathematically as a continuous or almost continuous mapping between two vectors X (input vector) and Y (output vector) and symbolically can be written as:

$$Y = M(X); \quad X \in \Re^n, Y \in \Re^m \tag{1}$$

where M denotes the mapping, n is the dimensionality of the input space (the number of NN inputs), and m is the dimensionality of the output space (the number of NN outputs). The simplest multi-layer perceptron (MLP) NN with one hidden layer and linear neurons in the output layer can be used as a generic analytical nonlinear approximation or model for the mapping (1) (Funahashi, 1989; Hornik, 1991). In our application, the possibility to use the simplest MLP NN is very important because the complexity and high dimensionality of the problem impose significant limitations on the arsenal of NN techniques and statistical metrics that can be used in our study. Also, the choice of statistical metrics used is determined and conditioned by those used for estimating errors and performances in the climate/weather modeling; this is a consequence of the interdisciplinary nature of the study.

The developed NN emulations for LWR and SWR are highly accurate and much more computationally efficient than the original NCAR CAM LWR and SWR, respectively. For example, the NN emulations using 50 neurons (NN50) for the LWR NN emulation and 55 neurons (NN55) for the SWR NN emulation in the single hidden layer provide, if run *separately* (code by code comparison) at every model physics time step (1 hour), the speed-up of $\sim$150 times for LWR and of $\sim$20 times for SWR as compared with the original LWR and SWR, respectively. These NNs have each more than 200 inputs and about 50 outputs (as many as the original LWR and SWR parameterizations which they emulate and substitute). The number of NN weights (or dimensionality of the NN training space) for these NNs reaches 10,000–20,000. The dimensionality is higher for NNs with a larger hidden layer and/or for models with higher vertical resolution (Krasnopolsky et al., 2005; Krasnopolsky, 2007).

All details of creating the training, validation, and test sets and of selecting the NN architecture are discussed in Krasnopolsky (2007). Here we only mention that each of these independent data sets consist of more than 100,000 records. Each record is a combination of an input vector X with more than 200 components and an output vector Y with about 50 components. Problems associated with normalizing multiple outputs of different nature and with choosing an error metric and a training algorithm, when dealing with such high-dimensional mappings and long training sets, are discussed in details in our earlier paper (Krasnopolsky & Fox-Rabinovitz, 2006).

The results of long multi-decadal climate simulations performed with NN emulations for both LWR and SWR, i.e., for the full model radiation, have been validated against the parallel control NCAR CAM simulation using the original LWR and SWR. Almost identical results have been obtained for these parallel 50-year climate simulations (Krasnopolsky, Fox-Rabinovitz, & Belochitski, 2007).

In another numerical model, an ocean wind wave model which is used for the simulation and forecast of ocean waves, the nonlinear wave–wave interaction represents a significant computational “bottleneck”. An accurate calculation of this component requires roughly 10^3–10^4 times more computational effort than all other aspects of the wave model combined.