PCE-PINNs: PHYSICS-INFORMED NEURAL NETWORKS FOR UNCERTAINTY PROPAGATION IN OCEAN MODELING

Björn Lütjens*, 1, Catherine H. Crawford2, Mark Veillette3, Dava Newman1
1Human Systems Laboratory, MIT, 2IBM Research, 3MIT Lincoln Laboratory

ABSTRACT

Climate models project an uncertainty range of possible warming scenarios from 1.5 to 5°C global temperature increase until 2100, according to the CMIP6 model ensemble. Climate risk management and infrastructure adaptation requires the accurate quantification of the uncertainties at the local level. Ensembles of high-resolution climate models could accurately quantify the uncertainties, but most physics-based climate models are computationally too expensive to run as ensemble. Recent works in physics-informed neural networks (PINNs) have combined deep learning and the physical sciences to learn up to 15k faster copies of climate submodels. However, the application of PINNs in climate modeling has so far been mostly limited to deterministic models. We leverage a novel method that combines polynomial chaos expansion (PCE), a classic technique for uncertainty propagation, with PINNs. The PCE-PINNs learn a fast surrogate model that is demonstrated for uncertainty propagation of known parameter uncertainties. We showcase the effectiveness in ocean modeling by using the local advection-diffusion equation.

1 INTRODUCTION

Informing decision-makers about uncertainties in local climate impacts requires ensemble models. Ensemble models solve the climate model for a distribution of parameters and initial conditions to generate a distribution of local climate impacts (Gneiting & Raftery, 2005). The physics of most oceanic processes can be well modeled at high-resolutions, but generating large ensembles is computationally too expensive: High-resolution ocean models resolve the ocean at 8 – 25km horizontal resolution and require multiple hours or days per run on a supercomputer (Fuhrer et al., 2018). Recent works are leveraging physics-informed deep learning to build “surrogate models”, i.e., computationally-lightweight models that interpolate expensive simulations of ocean, climate, or weather models (Rasp et al., 2018; Brenowitz et al., 2020; Yuval & O’Gorman, 2020; Kurth et al., 2018; Runge et al., 2019). The lightweight models achieve a acceleration the simulations on the order of 30 – 15k-times (Yuval & O’Gorman, 2020; Rackauckas et al., 2020). Building lightweight surrogate models could enable the computation of large ensembles.

The incorporation of domain knowledge from the physical sciences into deep learning has recently achieved significant success (Rassi et al., 2019; Steven L. Brunton, 2019; Rasp et al., 2018). Within physics-informed deep learning one could adapt the neural network architecture to incorporate physics as: inputs (Reichstein et al., 2019), training loss (Rassi et al., 2019), the learned representation (Lusch et al., 2018; Greidanus et al., 2019; Bau et al., 2020), hard output constraints (Mohan et al., 2020), or evaluation function (Lütjens* et al., 2021; Lesort et al., 2019). Alternatively, one could embed the neural network in differential equations (Rackauckas et al., 2020), for example, as: parameters (Garcia & Shigidi, 2006; Rassì et al., 2019), dynamics (Chen et al., 2018), residual (Karpate et al., 2017; Yuval et al., 2021), differential operator (Rassi et al., 2018; Long et al., 2019), or solution (Rassi et al., 2019). We embed a neural network architecture in the solution which will enable fast propagation of parameter uncertainties and sensitivity analysis.

* Corresponding email: lutjens@mit.edu
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While most work in physics-informed deep learning has focused on deterministic methods, recent methods explore the expansion to stochastic differential equations (Zhang et al., 2019; Dandekar et al., 2021; Yang et al., 2020; Zhu et al., 2019; Liu Yang, 2020). In particular, Zhang et al. (2019) achieves lightweight surrogate models for parameter estimation and uncertainty propagation by combining physics-informed neural networks (Raissi et al., 2019) with arbitrary polynomial chaos (Wan & Karniadakis, 2006). We use the simpler polynomial chaos expansion (Smith, 2013) instead of arbitrary polynomial chaos expansion, and focus on the task of uncertainty propagation in (Zhang et al., 2019). Further, we are the first in applying the combination of polynomial chaos and neural networks to the stochastic local advection-diffusion equation (ADE). Methods of uncertainty quantification have extensively been demonstrated on the local ADE (Smith, 2013); the advantage of neural networks is the ability to estimate PCE coefficients in high-dimensional spaces. The local ADE, also called horizontally averaged Boussinesq equation, is more challenging than the 1D stochastic diffusion equation from (Zhang et al., 2019) and illustrates the application to ocean modeling.

In summary our work contributes, PCE-PINNs, the first method for fast uncertainty propagation of parameter uncertainties with physics-informed neural networks in ocean modeling.

2 APPROACH

We are defining the initial value problem of solving the stochastic partial differential equation,

\[ \mathcal{N}(T(t, z; \omega); \kappa(z; \omega)) = 0, \quad t, z \in D, \omega \in \Omega, \]

B.C.: \[ B_{t, z}[T(t = 0, z; \omega)] = 0, \]

with spatial domain, \( D_z \), temporal domain, \( D_t \), random space, \( \Omega \), domain boundary, \( \Gamma \), nonlinear operator, \( \mathcal{N} \), and Dirichlet boundary conditions, \( B_{t, z} \).

2.1 DEFINING THE LOCAL ADVECTION-DIFFUSION EQUATION

We are given the local advection-diffusion equation which models the temperature distribution in a vertical ocean column over time,

\[ f = \frac{\delta T(t, z; \omega)}{\delta t} + \frac{\delta}{\delta z}(wT(t, z; \omega)) - \frac{\delta}{\delta z}\left(\kappa(z; \omega) \frac{\delta T(t, z; \omega)}{\delta z}\right) \]  

with height, \( z \in D_z = [0, 1] \), time, \( t \in D_t = [0, 1] \), source, \( f = 0 \), noise, \( \omega \in \Omega \), temperature, \( T : D_t, D_z \to \mathbb{R} \), stochastic diffusivity, \( \kappa(z, \omega) \), constant vertical velocity, \( w = 10 \).

We assume that the distribution over the diffusivity is known, for example, through data assimilation or Bayesian parameter estimation. Specifically, the diffusivity is assumed to follow an exponential Gaussian process (GP) with \( \kappa(z; \omega) = \exp(Y_\kappa(z; \omega)) \). The GP, \( Y_\kappa(z; \omega) \), is defined by mean,
\( \mu_{\gamma_e} = 1000 \), correlation length, \( L = 0.3 \), variance, \( \sigma_{\gamma_e} = 1.0 \), exponent, \( p_{\text{GP}} = 1.0 \), and a covariance kernel that is similar to the non-smooth Ornstein-Uhlenbeck kernel:

\[
\text{Cov}_{\gamma_e}(z_1, z_2) = \sigma_{\gamma_e}^2 \exp\left(-\frac{1}{p_{\text{GP}}} \left| \frac{z_1 - z_2}{L} \right|^p \right).
\]

### 2.2 Polynomial Chaos Expansion in Neural Networks

In practice, computing ensembles of differential equations such as in equation (1) for a distribution of parameter inputs is often computationally prohibitive. Hence, we aim to learn a copy, or fast surrogate model, of the differential equation solver, \( T : D_x \times D_z \rightarrow \mathbb{R} \), assuming a known parameter distribution and a set of ground truth solutions, \( T \in \mathbb{T} \), from the solver.

The polynomial chaos expansion (PCE) approximates arbitrary stochastic functions by a linear combination of polynomials (Smith [2013]). The polynomials capture the stochasticity by applying a nonlinear function to typically simple distributions and the coefficients capture the spatio-temporal dependencies (Smith [2013]). PCE has been widely adopted in computational fluid dynamics (CFD) community, because it offers fast inference time, analytical statistical summaries, such as \( C_0 = \mu_x \), and the theoretical guarantees of polynomials (Smith [2013]). However, the computation of PCE coefficients, \( \hat{C}(t, z) \), is analytically complex, because the computation differs among problems, and computationally expensive, because the computation involves integrals over the random space (Smith [2013]). Hence, we leverage neural networks to learn the PCE coefficients, \( \hat{C}(t, z) \), directly from observations of the solution.

The polynomial chaos expansion then approximates the solution as,

\[
\hat{T}(t, z; \vec{\xi}) = \sum_{j=0}^{\left| A \right|} \hat{C}_{\vec{\alpha}_j}(t, z) \Psi_{\vec{\alpha}_j}(\xi_1, \ldots, \xi_n) \tag{3}
\]

with the NN-based PCE coefficients, \( \hat{C}_{\vec{\alpha}}(t, z) \in \mathbb{R} \), the vector of polynomial degrees or multi-index, \( \vec{\alpha}_j \in A \) with \( j \in \{0, \ldots, \left| A \right| \} \), the set of multi-indices, \( A \), the maximum polynomial degree, \( n \), and the set of polynomials, \( \Psi_{\vec{\alpha}}(\vec{\xi}) \). The polynomials are defined by a set of multivariate orthogonal Gaussian-Hermite polynomials,

\[
\Psi_{\vec{\alpha}_j}(\xi_1, \ldots, \xi_n) = \Pi_{i=1}^n \psi_{\alpha_{j_i}}(\xi_i),
\]

\[
= \Pi_{i=1}^n \text{He}_{\alpha_{j_i}}(\xi_i),
\]

with \( \xi_i \sim \mathcal{N}(0, 1) \).

with the one-term (monic) polynomials, \( \psi_{\alpha_{j_i}} \) of polynomial degree, \( \alpha_{j_i} \). We are choosing the random vector of each stochastic dimension, \( i \in \{0, \ldots, n\} \), to be a Gaussian, \( \xi_i \sim \mathcal{N}(0, 1) \) and use the associated probabilists’ Hermite polynomials, \( \text{He}_{\alpha_{j_i}} \). The polynomial degrees are given by the total-degree multi-index set, \( A = \{ \vec{\alpha}_j \in \mathbb{N}_0^n : \|\vec{\alpha}_j\|_1 = \sum_{i=1}^n \alpha_{j_i} \leq n \} \). For example, \( A = \{ (0, 0), (0, 1), (1, 0), (1, 1), (2, 0), (0, 2) \} \) for \( n = 2 \). The number of terms, \( \left| A \right| \), is given by,

\[
\left| A \right| = \frac{(n+n)!}{n!n!}.
\]

The neural network (NN) then jointly approximates all PCE coefficients,

\[
\text{NN}_{C_A}(t, z) := \hat{C}_A(t, z) : D_t \times D_z \rightarrow \mathbb{R}^{\left| A \right|} \tag{5}
\]

The NN is trained to approximate PCE coefficients while only using the limited number of measurements, \( T \in \mathbb{R} \), as target data. The mean-squared error (MSE) loss function for episode, \( e \), and batch size, \( B \), is defined as:

\[
L_e(t_b, z_b) = \frac{1}{B} \sum_{b=1}^B \| T_b - \hat{T}_{\vec{\xi}_b} \|^2,
\]

\[
= \frac{1}{B} \sum_{b=1}^B \| T(t_b, z_b; \vec{\xi}_b) - \sum_{j=0}^{\left| A \right|} \hat{C}_{\vec{\alpha}_j}(t_b, z_b) \Psi_{\vec{\alpha}_j}(\vec{\xi}_b) \|^2,
\]

3
Initial results show that the PCE-PINNs in Fig. 2b can approximately match the mean (line) and standard deviation (shade) of the target solution in Fig. 2a with $MSE = 0.0078$. Importantly the approximated standard deviation also captures the growing trend towards the center location ($x = 0.5$) and growing time, $t = 1$.

where the realizations of random vectors, $\tilde{\xi}_b \sim \mathcal{N}(0, 1)^n$ are shared between the target and approximated solution. The batch size is chosen to fit one solution sample, $B = n_t n_z$ with t-grid size, $n_t$, and z-grid size, $n_z$.

3 RESULTS

Figure 2 shows that the PCE-PINNs in Fig. 2b can successfully approximate the mean and standard deviation of the target solution Fig. 2a. Importantly the explicit formulation as polynomial chaos expansion allows us to compute the mean and standard deviation without any sampling as a function of the PCE coefficients, e.g., $\mu_T(t, z) = C_0(0, 0, 0)(t, z)$. We can note that the PCE-PINN-approximated standard deviation captures the growing trend towards the center location ($x = 0.5$) and increasing time ($t = 1$). Quantitative analysis shows that the mean error is, as a sum over the full spatio-temporal domain, low $MSE = 0.0078$.

We observe that the PCE-PINNs slightly overestimate the uncertainty of the initial state (blue), have a marginal positive bias towards the right boundary ($x \approx 1$), and have lower curvature during the initial steps ($t \approx 0$). Future work will explore stronger constraints on satisfying the underlying physics equations and explore a broader choice of neural networks hyperparameters to further reduce the error.

We used a 2-layer 128-unit fully-connected neural network with ReLu activation. The network was trained with the ADAM optimizer with learning rate, $lr = 0.001$, and $\beta_1 = 0.9, \beta_2 = 0.999$ for $E = 15$ epochs. The target data was generated with $n_t = 128$ temporal and $n_z = 64$ grid points and $n_s = 100$ samples of the solved differential equation. The maximum polynomial degree was chosen to be, $n = 2$, s.t. the number of PCE coefficients, $|A| = 3$.

Leveraging neural network-based surrogate models can not only reduce computational complexity but also storage complexity. Our network contains $n_w = 2n_{units} + n_{layers}n_{units}^2 + n_{units}|A| = 33408$ weights which occupy as floats $n_{weights}AB \approx 133kB$.

4 DISCUSSION AND FUTURE WORK

We have demonstrated a novel technique for fast uncertainty propagation with physics-informed neural networks on the local advection-diffusion equation. The PCE-PINNs uses neural networks to learn the spatio-temporal coefficients of the polynomial chaos expansion, reducing the analytical and computational complexity of previous methods. Our method learned a lightweight surrogate model of the local advection-diffusion equation and successfully quantified the output uncertainties, given known parameter uncertainties.

We note that our results show room for improvement. Future work will explore stronger constraints on satisfying the physical laws in (1), e.g., via physics-based regularization terms (Raissi [2018]) or hard physics-constraints (Beucler et al. [2021]). Further, computational resources were limited during this experiment and future work will further optimize the choice of hyperparameters for the
neural network. Lastly, the proposed approach requires computation of a training dataset of solved differential equation for a set of parameter samples which can quickly become computationally expensive. Future work, will explore self-supervised learning approaches to enable learned surrogate models without the use of expensive training data.

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