Data-driven Equation Discovery of Ocean Mesoscale Closures

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Abstract

The resolution of climate models is limited by computational cost. Therefore, we must rely on parameterizations to represent processes occurring below the scale resolved by the models. Here, we focus on parameterizations of ocean mesoscale eddies and employ machine learning (ML), namely relevance vector machines (RVM) and convolutional neural networks (CNN), to derive computationally efficient parameterizations from data, which are interpretable and/or encapsulate physics. In particular, we demonstrate the usefulness of the RVM algorithm to reveal closed-form equations for eddy parameterizations with embedded conservation laws. When implemented in an idealized ocean model, all parameterizations improve the statistics of the coarse-resolution simulation. The CNN is more stable than the RVM such that its skill in reproducing the high-resolution simulation is higher than the other schemes; however, the RVM scheme is interpretable. This work shows the potential for new physics-constrained interpretable ML turbulence parameterizations for use in ocean climate models.

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Key Points:

- We present two machine learning algorithms for ocean mesoscale parameterizations.
- We discover closed-form equations for eddy momentum, temperature and energy parameterizations.
- Deep learning closure is more stable than closed-form equations when implemented in an ocean model.

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Abstract

The resolution of climate models is limited by computational cost. Therefore, we must rely on parameterizations to represent processes occurring below the scale resolved by the models. Here, we focus on parameterizations of ocean mesoscale eddies and employ machine learning (ML), namely relevance vector machines (RVM) and convolutional neural networks (CNN), to derive computationally efficient parameterizations from data, which are interpretable and/or encapsulate physics. In particular, we demonstrate the usefulness of the RVM algorithm to reveal closed-form equations for eddy parameterizations with embedded conservation laws. When implemented in an idealized ocean model, all parameterizations improve the statistics of the coarse-resolution simulation. The CNN is more stable than the RVM such that its skill in reproducing the high-resolution simulation is higher than the other schemes; however, the RVM scheme is interpretable. This work shows the potential for new physics-constrained interpretable ML turbulence parameterizations for use in ocean climate models.

Plain Language Summary

The complexity of numerical models used for future climate projections is limited by their computational cost. Many key processes, such as ocean eddies, are not adequately resolved and must be approximated using parameterizations. However, parameterizations are often imperfect and reduce the accuracy of the simulations. Machine learning is now opening new avenues to improve climate simulations by extracting such parameterizations directly from data, rather than using idealized theories as typically done. We show that efficient modern machine learning algorithms can accurately represent the physics of ocean eddies, be constrained by physical laws, and can be interpretable. Our results simultaneously open the door to the discovery of new physics from data and the improvement of climate simulations.

1 Introduction

Turbulent processes are critical components of the climate system and influence the circulation of both the ocean and atmosphere. For example, ocean mesoscale eddies, which are turbulent features of scale 10-100 km, dominate the oceanic kinetic energy reservoir (Ferrari & Wunsch, 2009) and are key for the lateral and vertical transport of tracers, such as heat, carbon, and oxygen. These turbulent processes occur on scales that are below the resolution of typical global climate models, which is roughly 25 km-100 km (IPCC, 2013). Therefore, the effects of these turbulent processes on the large-scale must be approximated.

These approximations, called parameterizations or closures, are often developed using idealized theories of the bulk effect of the subgrid process on the large scale (Warner, 2010). This approach has been used for many decades but is not necessarily optimal as it neglects certain physical effects. Imperfections in current parameterizations and missing physics in climate models introduce significant biases in simulations and considerable uncertainty in anthropogenic climate change projections (IPCC, 2013). For example, current parameterizations of ocean eddies target the effect of i) buoyancy fluxes by removing large-scale available potential energy (Gent & Mcwilliams, 1990), and ii) momentum fluxes using viscous closures which dissipate momentum (Zanna et al., 2020).

While improving certain properties of the flow (Danabasoglu et al., 1994), eddy parameterizations are missing key energy pathways such as the conversion of available potential energy into subgrid kinetic energy, or the backscatter of kinetic energy to the large-scale flow (Jansen et al., 2015; Zanna et al., 2017; Bachman, 2019). In addition, these parameterizations spuriously dissipate kinetic energy (Jansen & Held, 2014; Kjellsson

& Zanna, 2017). These imperfect representations of ocean eddy physics in models can affect the strength and variability of large-scale ocean currents and ocean heat uptake (Zanna et al., 2017; Kuhlbrodt & Gregory, 2012). Increasing resolution can reduce some of these biases; however, due to the computational expense of running turbulence-resolving simulations, subgrid parameterizations will be in demand for several decades.

Recently, the advent of machine learning (ML) has given rise to a new class of data-driven parameterizations. Studies rely on ML to optimally tune parameters of existing closures (Schneider et al., 2017; Ling et al., 2016). This approach, while useful, still neglects the missing physics not encapsulated in the current parameterizations. Instead, several studies have shown the promise of new ML parameterizations of subgrid processes in the atmosphere (Gentine et al., 2018; Rasp et al., 2018; O'Gorman & Dwyer, 2018; Brenowitz & Bretherton, 2018) and ocean (Bolton & Zanna, 2019). However, this new class of ML parameterizations often uses black-box algorithms (e.g., neural networks) such that the laws of physics are not necessarily respected unless imposed (Beucler et al., 2019; Ling et al., 2016), and interpreting the data-driven parameterization becomes intractable.

Here, we propose a complementary or alternative route to both the traditional physics-driven bulk approach and the ML-black box approach of deep learning. We use ML to discover closed-form equations for mesoscale eddy parameterizations for coarse-resolution ocean models using high-resolution model data. Given some spatio-temporal dataset of the subgrid eddy forcing, we uncover an equation that could have produced that dataset (Rudy et al., 2017; Zhang & Lin, 2018). This approach has the following advantages over more complex methods such as convolutional neural networks: the end result is significantly easier to interpret physically, the computational cost of implementation is lower, and training time of the algorithm is also lower. Data-driven discovery of equations has been extensively used to reveal known-equations, such as Burger's or Navier-Stokes' equations (Kutz, 2017). However, unlike in these studies, we use the algorithm to discover unknown equations for the subgrid eddy forcings.

2 Data and Methods

2.1 Training Data and Coarse-Graining

We use a primitive equation model, MITgcm (J. Marshall et al., 1997), to generate high-resolution data and construct new eddy momentum, temperature and energy parameterizations. We run highly-idealized double-gyre eddy-resolving barotropic and baroclinic simulations in a square-domain. The simulations use a beta-plane approximation, free-slip boundary conditions on lateral walls and no-slip boundary condition on the bottom, and a constant surface zonal wind forcing. These simulations are designed to create highly turbulent flow regimes, with mesoscale eddies shedding from the jet extension.

The barotropic model has a single layer of depth 500 m and length 3840 km, similar to Cooper and Zanna (2015). We spin-up the model from rest for 10 years, at a spatial resolution of 3.75 km. The baroclinic model comprises of 15 vertical levels, with a total depth of 3600 m. Due to the increased computational cost of running the baroclinic simulation compared to the barotropic model, we decreased the domain size from 3840 km in length to 1920 km, with a spatial resolution of 7.5 km. The meridional temperature gradient is imposed via surface restoring to a linear profile. We spin-up the baroclinic model for 100 years and then run for a further 10 years for data collection. Further details about the simulations are given in the Supplementary Information (SI, S1).

After spin-up, we select 1000 time-slices of model output, with 4 days between each time-slice. We remove information at small-scales by applying a horizontal Gaussian filter of width 30 km, and then coarse-grain to a 30 km grid, which is denoted by $\overline{(..)}$ (Bolton

& Zanna, 2019) (SI, S2). The subgrid eddy momentum and temperature forcing terms, for each vertical level, are then defined by

$$\mathbf{S_u} = \begin{pmatrix} S_x \\ S_y \end{pmatrix} = (\overline{\mathbf{u}} \cdot \overline{\nabla})\overline{\mathbf{u}} - \overline{(\mathbf{u} \cdot \nabla)\mathbf{u}}, \tag{1}$$

$$S_T = (\overline{\mathbf{u}} \cdot \overline{\nabla})\overline{T} - \overline{(\mathbf{u} \cdot \nabla)T}, \tag{2}$$

respectively. Here ∇ is the horizontal 2D gradient operator, T is the temperature, and the horizontal velocity $\overline{\mathbf{u}} = (\overline{u}, \overline{v})$. These terms reflect the turbulent nonlinear terms truncated in coarse-resolution models which need to be parameterized (Berloff, 2005; Mana & Zanna, 2014). At every grid-point for every time-slice, we both i) calculate the target eddy forcing, i.e, Eqs. (1) and (2), and ii) construct a library of diverse functions which are necessary for the RVM method described below and are relevant to the process being parameterized.

2.2 Data-Driven Algorithms

Relevance Vector Machine. Here, we employ the sparse Bayesian regression method used in Zhang and Lin (2018) based on relevance vector machines (RVM) (Tipping, 2001) to reveal new eddy parameterizations. RVM is a regression technique that assumes Gaussian prior distributions for each regression weight (Bishop, 2006). The width of the Gaussian prior of each regression weight provides a measure of uncertainty of that regression weight. The method relies on a library of functions, which can comprise of any function such as products or derivatives of relevant quantities defined as basis functions (e.g., velocity shears, temperature shears). The sparse regression is applied iteratively to the library of functions, and then a pruning of the library of functions is carried out by discarding the functions with an uncertainty higher than a pre-specified threshold (Zhang & Lin, 2018). This uncertainty threshold, δ, is the only parameter that requires setting in the Zhang and Lin (2018) method. The algorithm finishes when the uncertainty measures of each regression weight stop changing from iteration to iteration. We found the Zhang and Lin (2018) method to be more robust than the sequential threshold ridge regression (STRidge) of Rudy et al. (2017). For example, using data to discover the known 2D advection-diffusion equations, we found that STRidge required substantially more data for training than the RVM method, STRidge has a large number of tunable hyperparameters which substantially influenced the discovered equation compared to the RVM method which has only one hyperparameter. In addition, unlike STRidge, Zhang and Lin (2018) method provided an error associated with the weights discovered. Given these tests were performed on known equations in which we knew the answers, we opted for the use of Zhang and Lin (2018) RVM method to discover unknown parameterizations.

At every grid-point for every time-slice from the MITgcm coarse-grained output (described above) we construct a library of diverse functions, ϕ_i, which are derived from a set of basis functions relevant to the process being parameterized. We build the library from the filtered velocities $\overline{u}$, $\overline{v}$, and $\overline{T}$ using up to second-order for both spatial derivatives and polynomial products, mainly due to memory limitations. The basis of functions used for the momentum and temperature eddy parameterizations differ and will be discussed in the next section. We normalized each function individually such that they have zero mean and unit variance. We use 50% of the 1000 time-slices for training and the other 50% for validation. For both the eddy momentum and temperature forcing, we impose a physical constraint for global conservation. To do so, we only specify library functions that can be written as the divergence of a flux (or as the divergence of a tensor $\mathbf{T}$ for the eddy momentum forcing, i.e. $\overline{\nabla} \cdot \mathbf{T}$), such that with the appropriate boundary conditions there is no net input of momentum or temperature.

We then apply the iterative RVM algorithm to prune the library of functions and construct the final equation for the subgrid forcing (independently for S_x, S_y and S_T) as a linear sum of the functions, ϕ_i, each weighted by the regression coefficient, w_i. We

Figure 1. A) Illustration of the RVM procedure; B) Schematic of the architecture of the physics-constrained fully-convolutional neural network (FCNN); C) O ine validation of the sub-grid momentum forcing from the barotropic simulations for three parameterizations, denoted as $\hat{S}$ { the physics-driven $\hat{S}^{AZ}$, $\hat{S}^{BT}$ revealed by the RVM algorithm (Eq. 5), and the FCNN { against the diagnosed forcing from high-resolution data, S. Top Row shows the mean [ms ^{2}], Middle Row the Standard Deviation [ms ^{2}], and the Bottom Row the Pearson correlation of the zonal component of the eddy momentum forcing, S_x and $\hat{S}_x$ (the meridional component is shown in SI). The x- and y-axis are longitude and latitude, respectively; the extent is 3840 km in each direction.