No Free Lunch: How ML can be used (or misused) to uncover dynamical regimes in the ocean and beyond

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Overview: Minitutorial in two parts

- **Part 1: The ocean's role within climate and the data revolution**
- **Part 2: Dynamical regime discovery and interpretable/explainable ML**

Practical:
Exploring dynamical regime identification in a global oceanographic setting.

launch binder

https://github.com/maikejulie/MLINT

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Part 1: The ocean's role within climate and the data revolution

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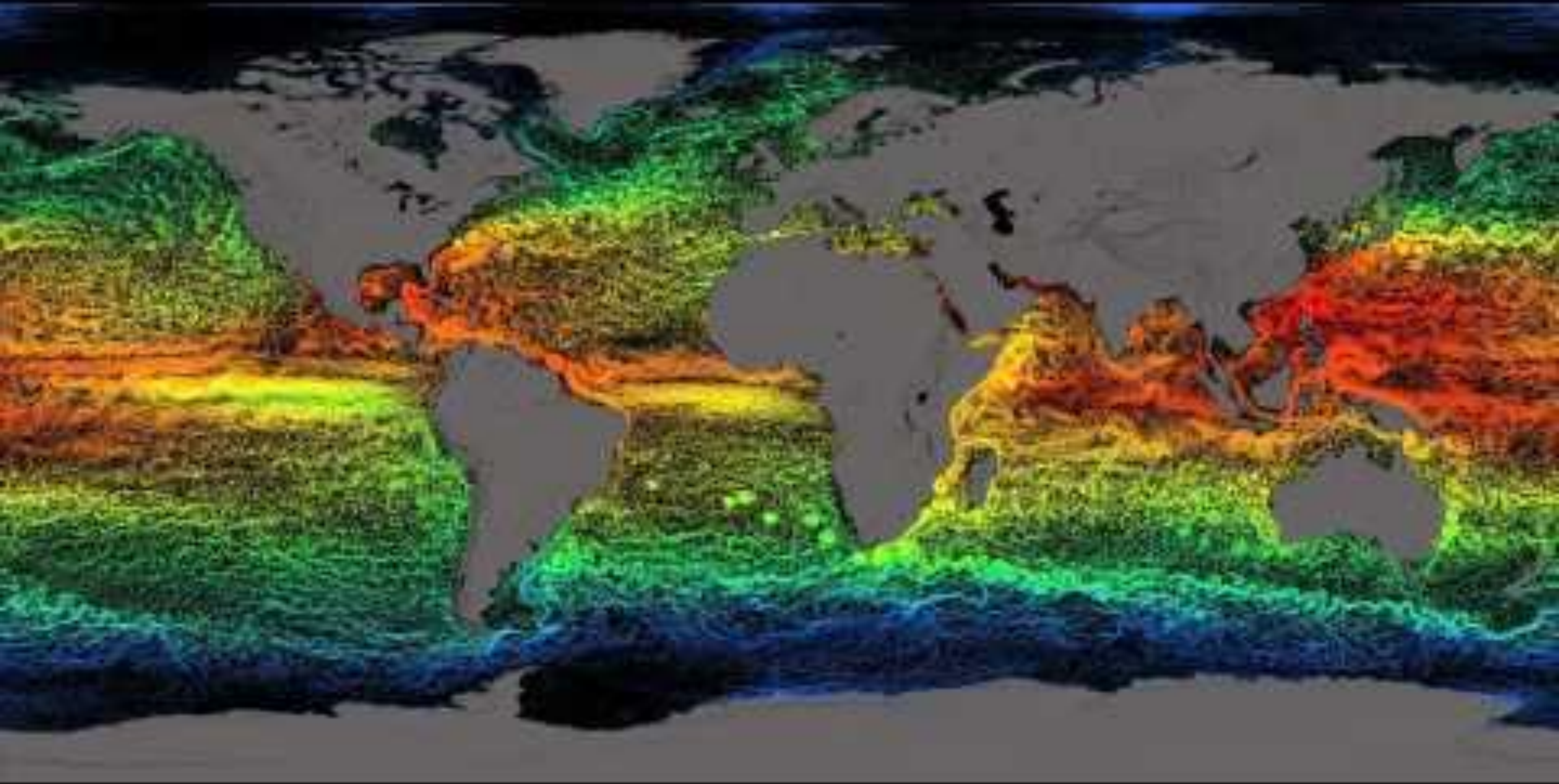
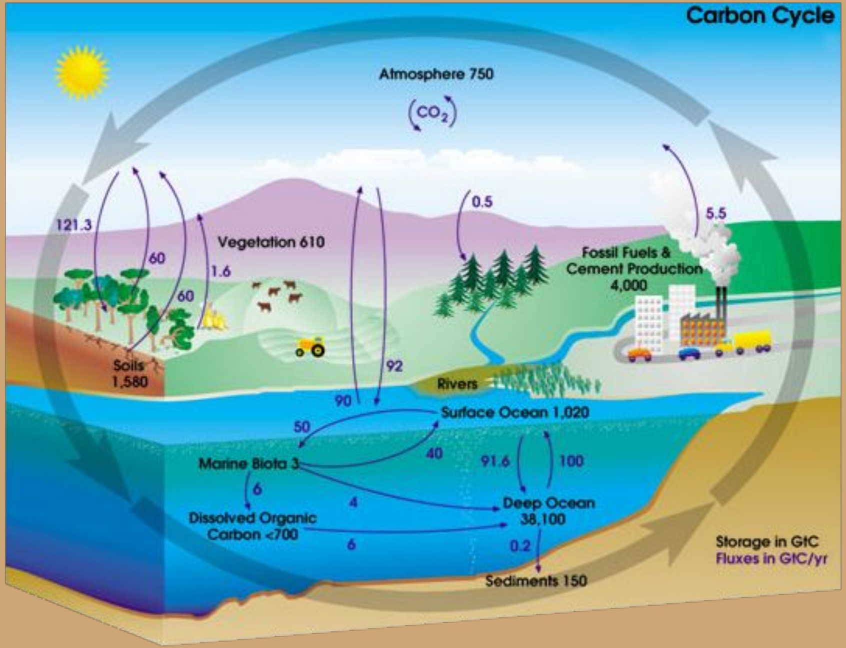
Review paper: Sonnewald et al. 2021, Bridging observation, theory and numerical simulation of the ocean using Machine Learning



The role of the ocean in the climate system

Carbon and heat storage



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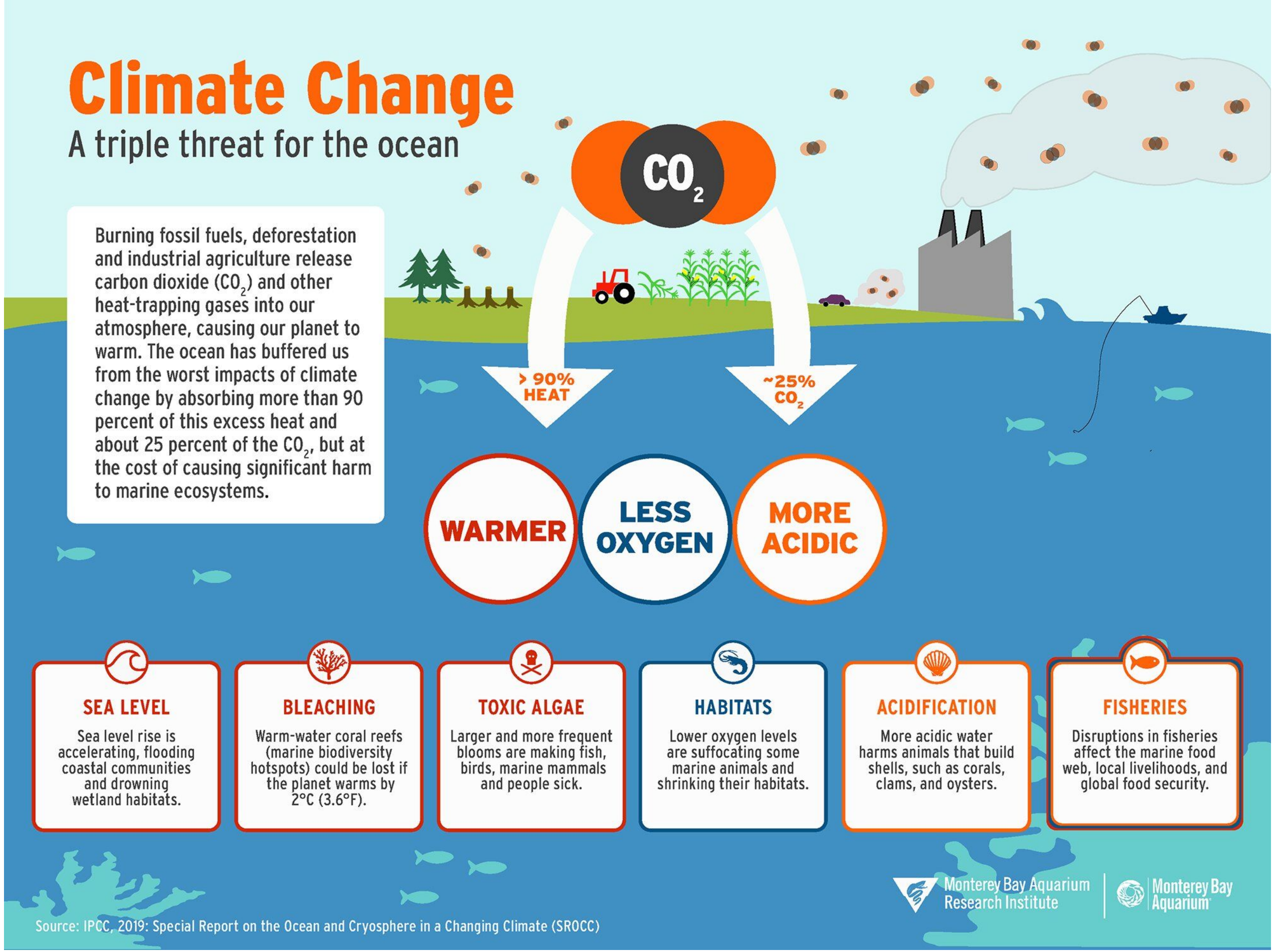
Climate change impacts society
Chaser.au



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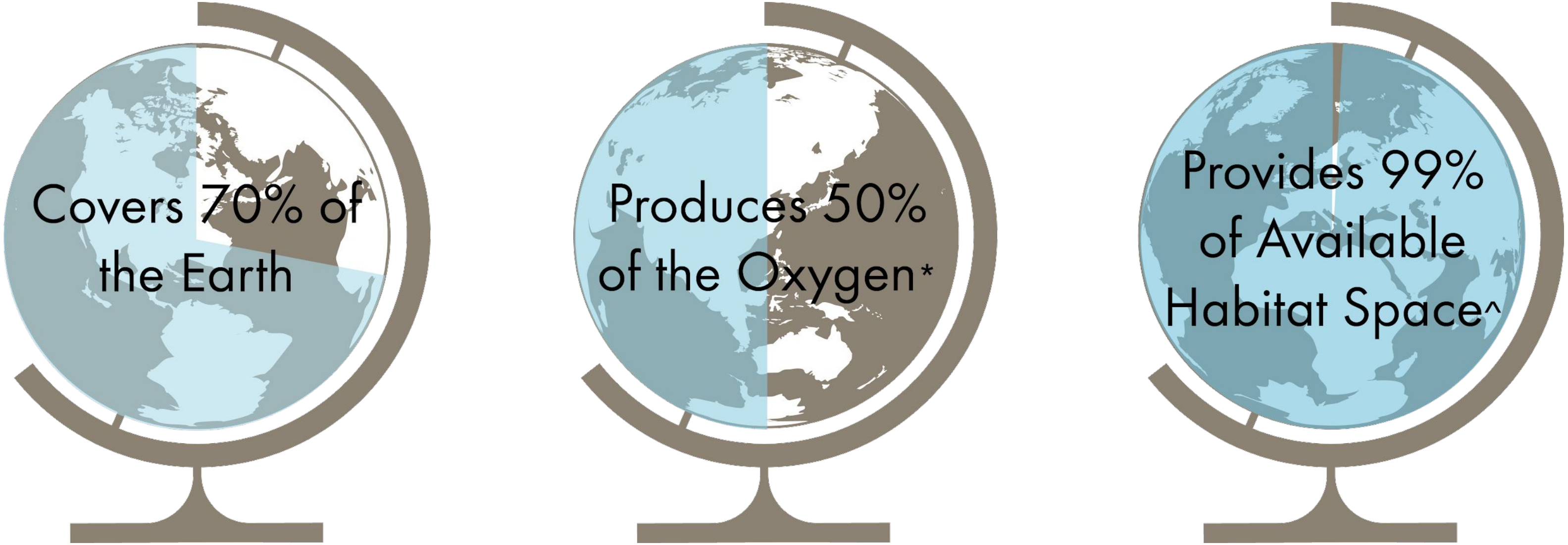
Services the ocean provides

The ocean, due to its large heat capacity, has absorbed more than 90% of the heat gained by the planet between 1971 and 2010.

Zanna 2019



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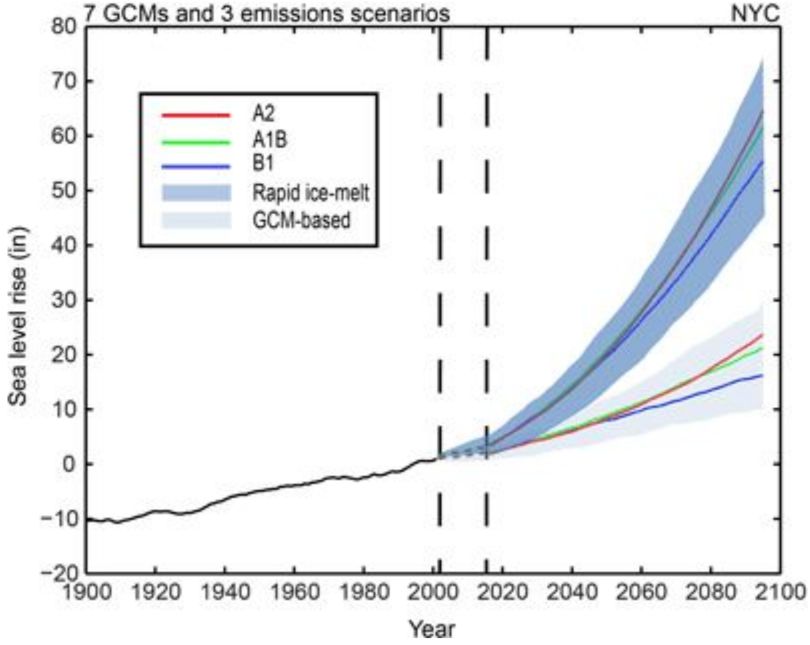
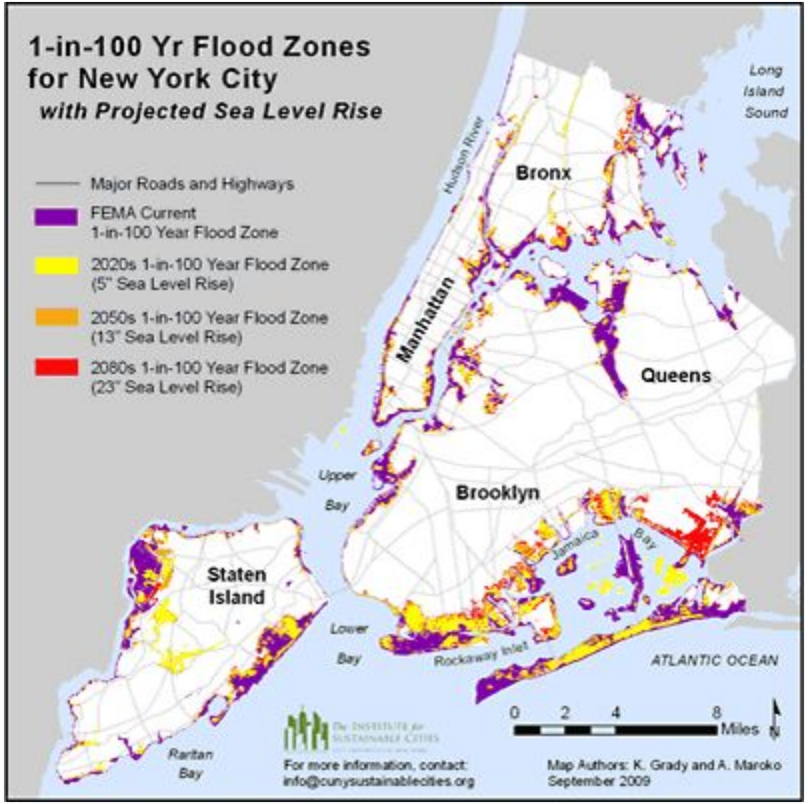
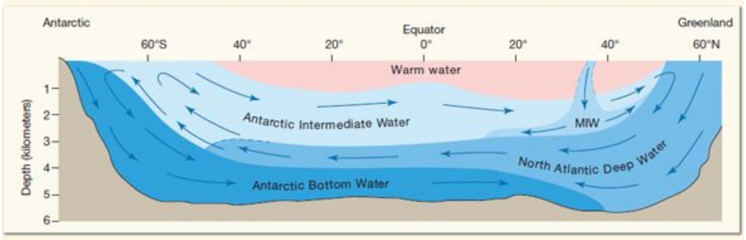
Ocean in a changing climate



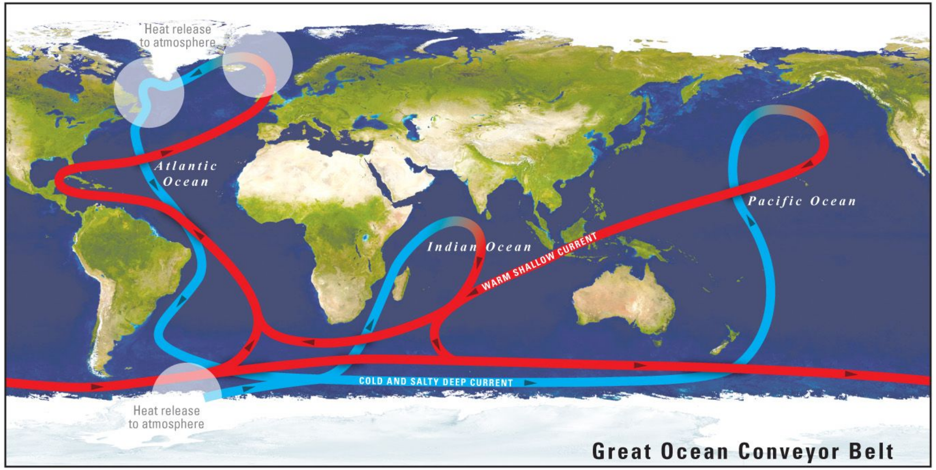


https://www.giss.nasa.gov/research/briefs/rosenzweig_03/

The ocean in Motion: A global “conveyor”



- The ocean is layered with the heaviest/densest water at the bottom
- Intense cooling and ice formation at the poles create very dense waters



- Asymmetrical heating/cooling, along with brine rejection from ice formation create the Thermohaline circulation
- Referred to as the ‘meridional overturning circulation’

Changes in overturning circulation have **big** climate impact

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Governing equations

Variations in T and S have profound influence on circulation

Mass

$$\rho^{-1}\frac{D\rho}{Dt} + \nabla \cdot \mathbf{u} = 0$$

$$\mathbf{u} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$$

Momentum

1&2 Navier-Stokes

$$\underbrace{\frac{D\mathbf{u}}{Dt}}_{\text{total accel.}} + \underbrace{2\boldsymbol{\Omega}\times\mathbf{u}}_{\text{Coriolis accel.}} = \underbrace{-\rho^{-1}\nabla p}_{\text{press grad}} - \mathbf{g} + \underbrace{\nu\nabla^2\mathbf{u}}_{\text{molecular dissip.}}$$

$\boldsymbol{\Omega}$ is the rotation vector of the earth

Heat

$$\frac{\rho T c_p}{\theta}\frac{D\theta}{Dt} = \nabla \cdot (k\nabla T - \mathbf{F}^{\mathrm{rad}}) + Q_H$$

c_p is the specific heat capacity

$\mathbf{F}^{\mathrm{rad}}$ is the vector of radiation

Q_H is heating due to phase changes

Salt

$$\rho\frac{DS}{Dt} = \nabla \cdot (\rho\kappa_D\nabla S)$$

κ_D is the diffusivity

$$\rho = \rho(p, S, \theta).$$

ρ is density; p is pressure; T is temperature; S is salinity

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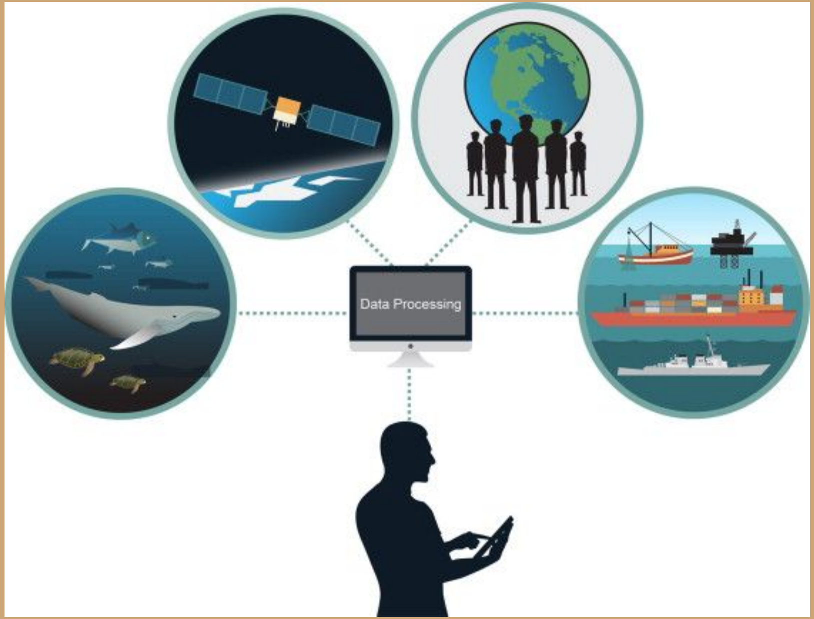
A data revolution, or a data problem?

Data rich and insight poor



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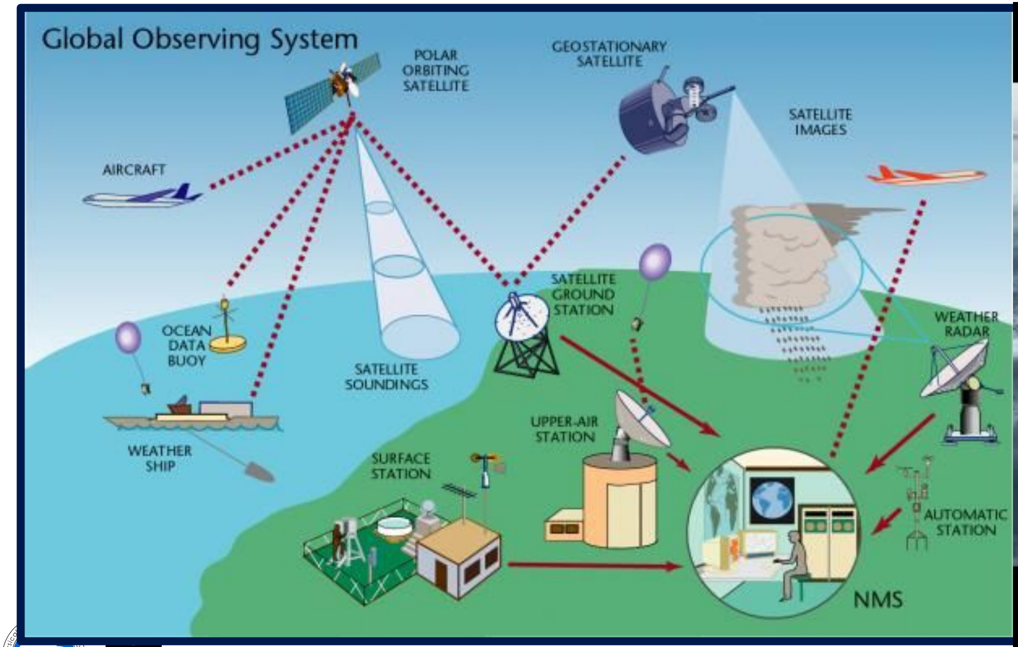
Ocean data: Observations



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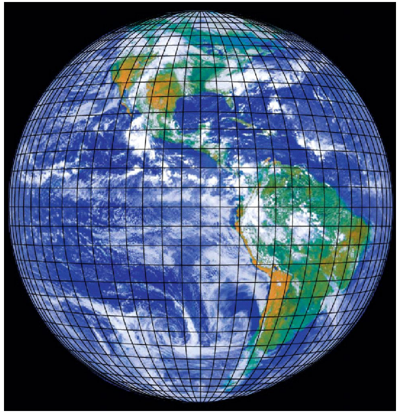
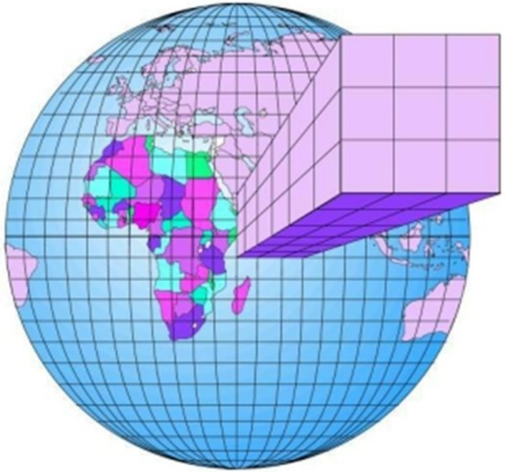
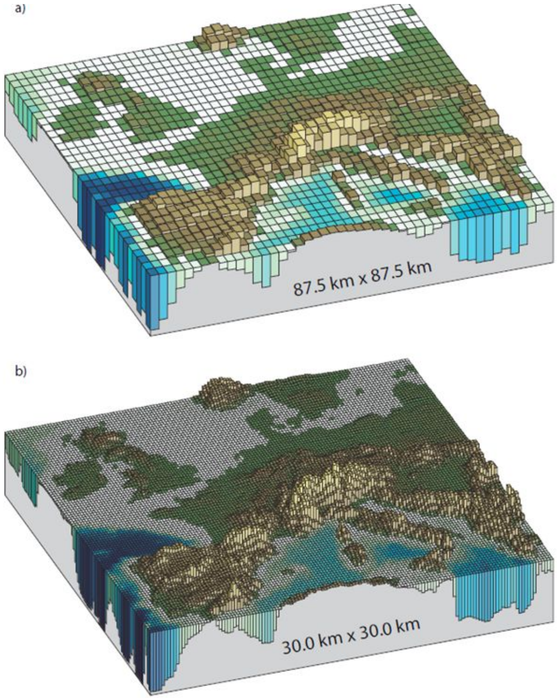
Ocean data: Numerical models

Just like your television, higher resolution means more realism







Grids extend downward into the land surface and oceans.

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Simulations: Primitive equations

Navier-Stokes + equation of state: Thin rotating fluid on a sphere

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} - fv = -\frac{1}{\rho_o}\frac{\partial P}{\partial x} + \frac{\partial}{\partial z}\left(K_m\frac{\partial u}{\partial z}\right) + F_u, \quad \text{Momentum (u component)}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} + fu = -\frac{1}{\rho_o}\frac{\partial P}{\partial y} + \frac{\partial}{\partial z}\left(K_m\frac{\partial v}{\partial z}\right) + F_v \quad \text{Momentum (v component)}$$

$$\frac{\partial P}{\partial z} = -\rho g, \quad \text{density}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \quad \text{continuity}$$

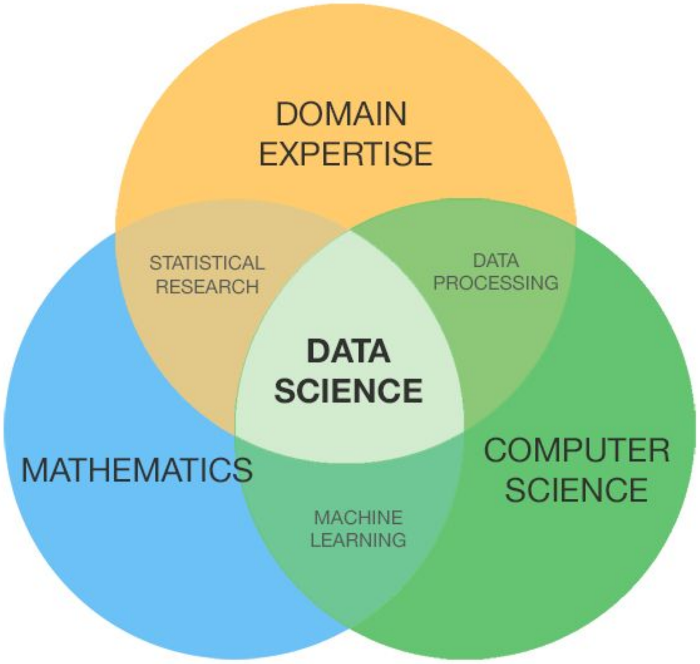
$$\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} + w\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z}\left(K_h\frac{\partial \theta}{\partial z}\right) + F_\theta, \quad \text{Advection of temperature}$$

$$\frac{\partial s}{\partial t} + u\frac{\partial s}{\partial x} + v\frac{\partial s}{\partial y} + w\frac{\partial s}{\partial z} = \frac{\partial}{\partial z}\left(K_h\frac{\partial s}{\partial z}\right) + F_s, \quad \text{Advection of salinity}$$

$$\rho = \rho(\theta, s), \quad \text{Density as a function of S and T}$$

Machine Learning for oceanography

Part of a bigger picture



Source: Palmer, Shelly. Data Science for the C-Suite.
New York: Digital Living Press, 2015. Print.

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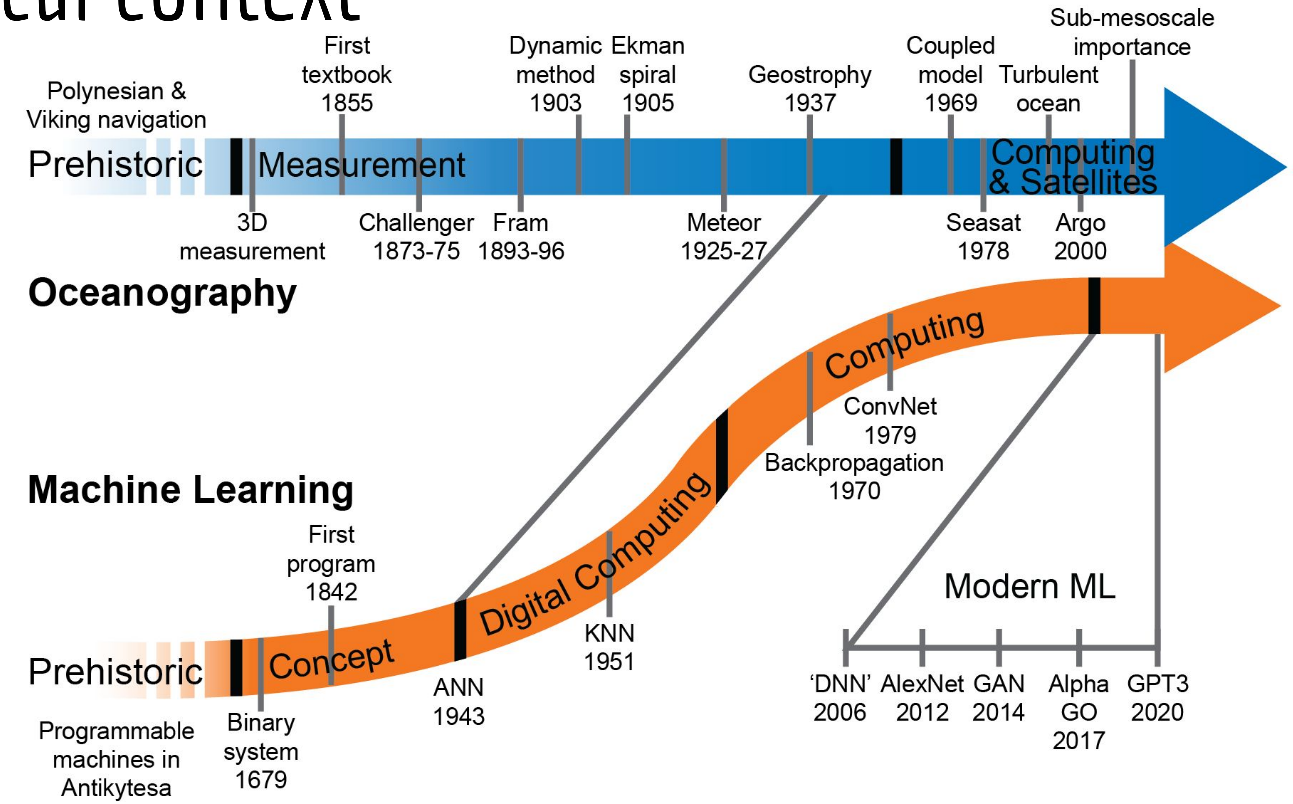
Historical context



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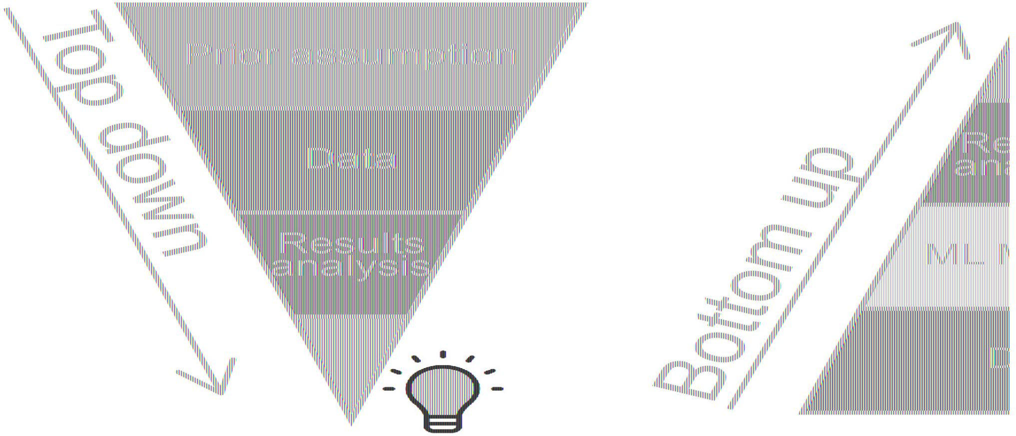
ML: The missing piece?

Too simple:
Theoretical descriptions of circulation tend to be oversimplified.

Too hard:
Interpreting basic physics from realistic/accurate models is hard.

Missing piece: ML



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ML within oceanography

Observations → Theory → Models → Predictions → Decision Support

Observations
- Observation operators
- Gap filling
- Error detection and bias correction
- Synthesis of observations
- In situ feature detection

Theory
- Learn equations and boundary conditions
- Unsupervised learning to understand dynamics and causality
- Learn process interactions
- Learn sub-grid-scale representation of models

Models
- Learn low-order models
- In situ updates of boundary conditions
- Speed-up simulations via emulation and preconditioning
- Compare models against observations
- Uncertainty quantification

Predictions
- Data assimilation
- Error correction
- Down-scaling
- Understand climate response
- Improve signal-to-noise
- In situ alarm systems

Decision Support
- Alarm systems
- Climate mitigation
- Route planning
- Oil spilling
- Flooding

Some are hopes...
others already implemented

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Hopes for ML

Increases the efficiency of research

Find patterns to accelerate exploration

Emergence of complex interactions

Allow processing of “big” data

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ML basics

Supervised

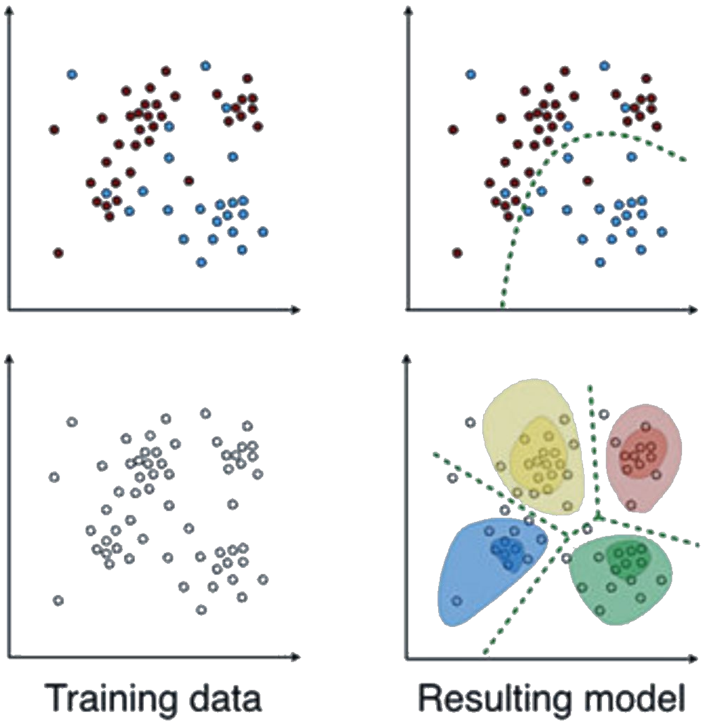
-Labeled data

-Decision boundary

Unsupervised

-No labels

-Identify structures



"If machine learning is a cake, then unsupervised learning is the actual cake, supervised learning is the icing, and RL is the cherry on the top."

Yann LeCun, DL pioneer at NeurIPS 2016

Supervised learning

$$\theta^* =[\ \theta] \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}\left(f\left(x^{(i)};\theta\right), y^{(i)}\right)$$

- Dataset of N input-output pairs $\{(x^{(i)}, y^{(i)})\}_{i\in 1..N}$
- Loss function $\mathcal{L}$ for discrepancy of prediction and actual outputs
- Parameters θ of the ML model f are found by optimization

If differentiable use of gradient based solver:

$$\theta_{k+1} = \theta_k - \mu \nabla \mathcal{L}\left(\theta_k\right),$$

where μ is the rate of descent/"learning rate" and ∇ the gradient operator.

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Supervised learning in brief

- Neural Networks (NN):
    - Universal approximators with interconnected nodes
- Random Forests (RF):
    - Composited of Decision Trees (DTs), or tree-like compositions of decision rules
- Support Vector Machine (SVM):
    - Find linear separating hyperplane
    - `Kernel trick’ popular: Not linear? Project onto higher dimensional plane!
- k-Nearest Neighbours:
    - Find closest points wrt a metric in the input data, classify by plurality vote

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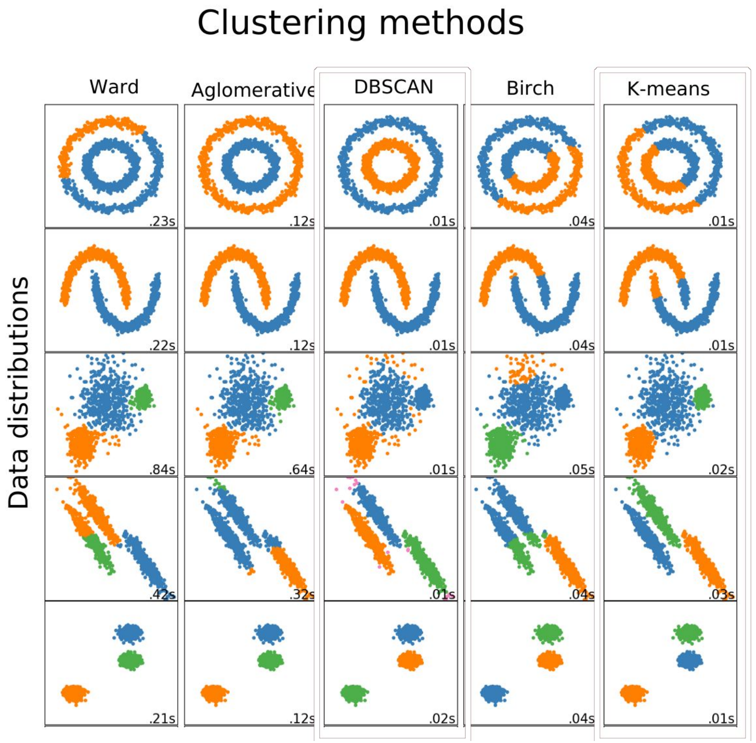
Unsupervised learning: Clustering

- Find patterns in data distributions
- Humans are excellent at pattern recognition in 2-3D
    - Machines can do ND

Other unsupervised methods: Anomaly detection



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How Much Information is the Machine Given during Learning?

Y. LeCun

- **"Pure" Reinforcement Learning (cherry)**
  - The machine predicts a scalar reward given once in a while.
  - **A few bits for some samples**
- **Supervised Learning (icing)**
  - The machine predicts a category or a few numbers for each input
  - Predicting human-supplied data
  - **10→10,000 bits per sample**
- **Self-Supervised Learning (cake génoise)**
  - The machine predicts any part of its input for any observed part.
  - Predicts future frames in videos
  - **Millions of bits per sample**

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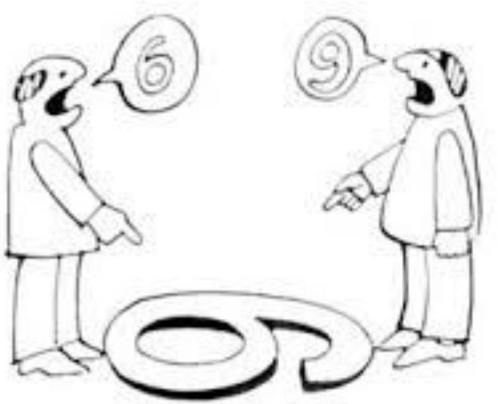
What ML methods are used where?

- Unsupervised: Exploring data and theory, decision support
- Supervised: Model development, physics constraints, bias & error correction, data assimilation
- No hard boundaries for methods applications
  - Deep learning used for data interpolation
  - 'Unsupervised' methods used to support supervised
- See much cross-pollination
- Constantly evolving



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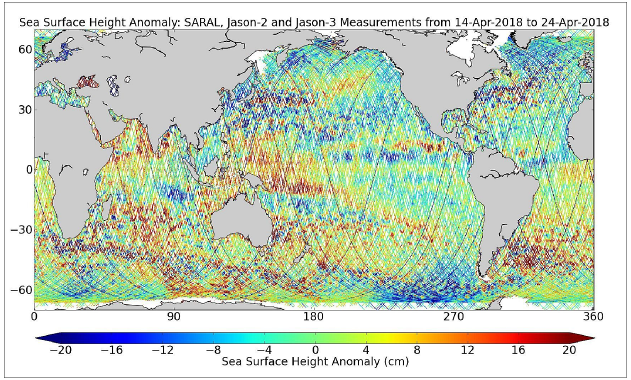
ML in observations: Satellites



- Satellite data offers unique global perspective
- Some have different orbits, and observe different variables e.g. sea surface temperature, salinity or velocity
- ML is used to fuse satellite products (Guiliambard et al, 2012)
- One can extract geophysical information, e.g. currents at 1000m (Duncan et al. 2019, Castelani 2006)
- ML can also be used to fuse satellite and in-situ data (Chapman & Alexandre, 2017, Mustapha et al. 2014, Denvil-Sommer, 2019)

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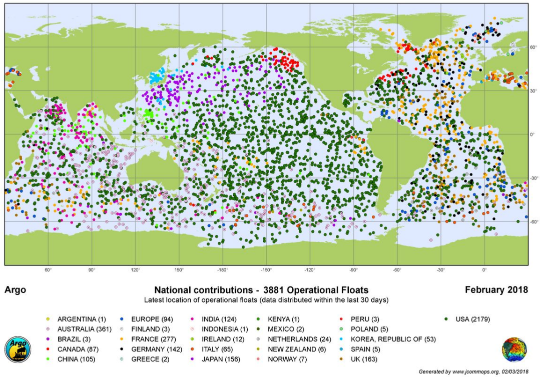
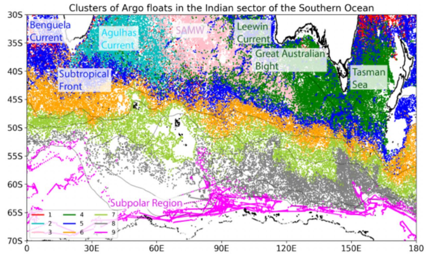
ML in observations: In-situ sampling

- In-situ sampling refers to data measured from the ocean directly, rather than remotely
- Vast amounts of data exist, but paradoxically there is e.g. almost no data from the deep ocean
- ML often used to extract patterns or`mine' in-situ data:
    - Objective assessment
- Areas of use:
    - Surface mixed layers (Maze et al. 2017)
    - Southern Ocean structures (Jones et al. 2019, Rosso et al. 2020)
- Detecting global modes:
    - El Nino Southern Oscillation (Hughton & Wilson 2020)





Science mag

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K-means

cluster guess, data, Distance function

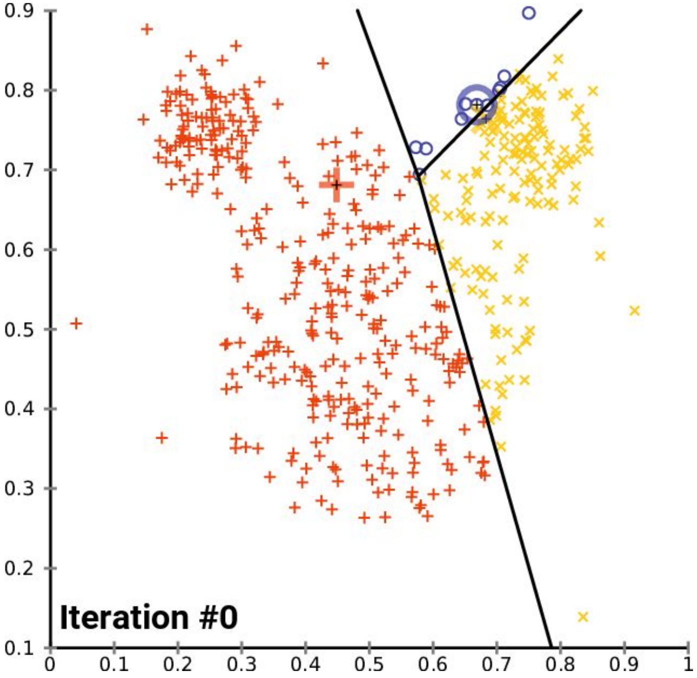
$$J = \sum_{j=1}^{k} \sum_{i=1}^{n} \overbrace{\|x_i^{j} - c_j\|^2}^{\text{Distance function}}$$

data point, centroids

Minimize objective function

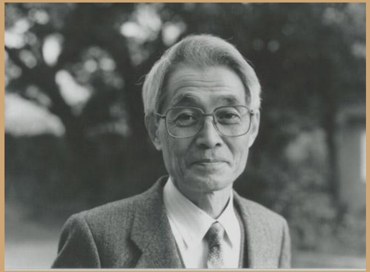
Setting **k** the number of clusters

Stochastic first guess



Finding the appropriate **k** is critical

Hirotugu Akaike
Gave us 'information criteria'



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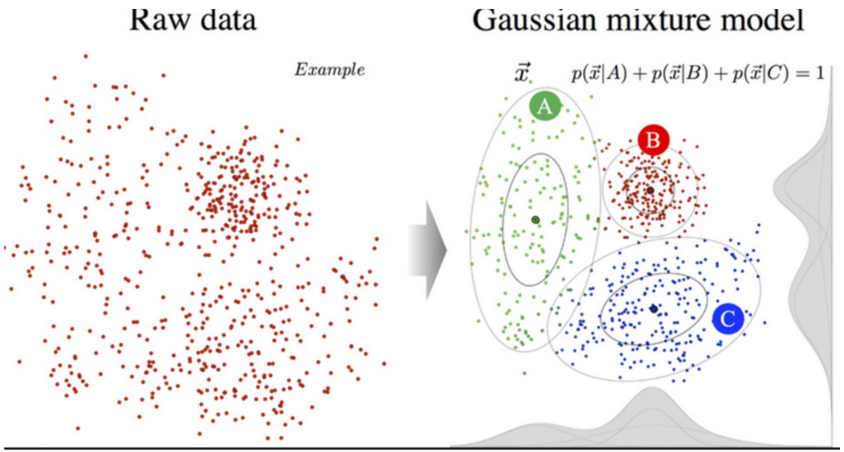
GMM

- GMM: the weighted sum of a number of Gaussians where the weights are determined by a distribution, π

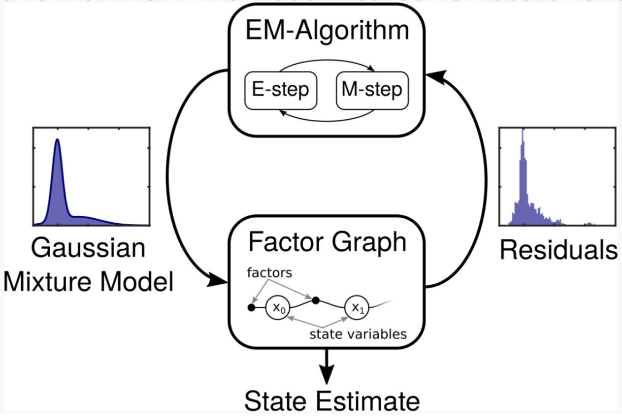
$$p(x) = \pi_0 N(x|\mu_0, \Sigma_0) + \pi_1 N(x|\mu_1, \Sigma_1) + \ldots + \pi_k N(x|\mu_k, \Sigma_k)$$

$$\text{where } \sum_{i=0}^{k} \pi_i = 1$$

$$\boxed{p(x) = \sum_{i=0}^{k} \pi_i N(x|\mu_k, \Sigma_k)}$$



Iterative maximum likelihood method for latent variables



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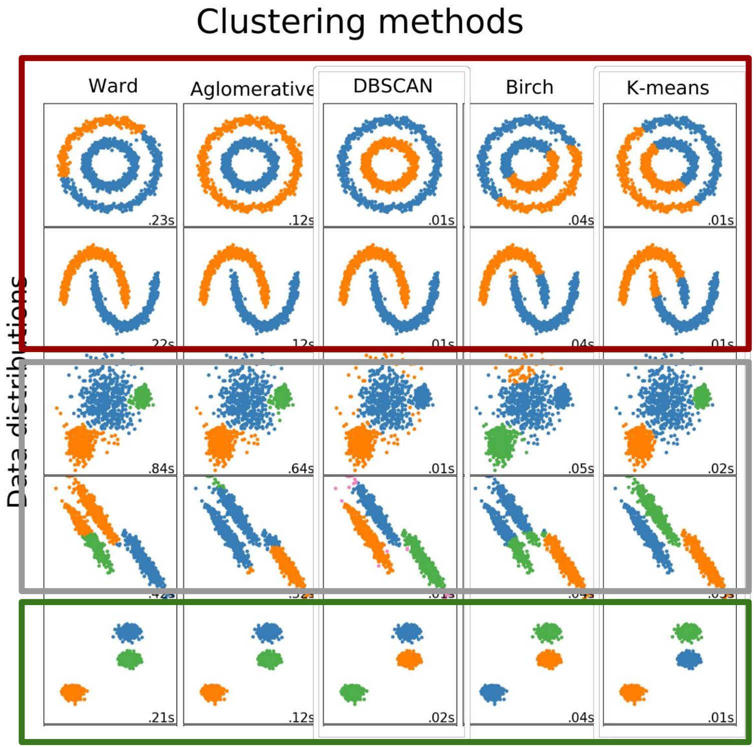
Ocean data need not have a normal distribution



<- Non-Gaussian!

Gaussian ->

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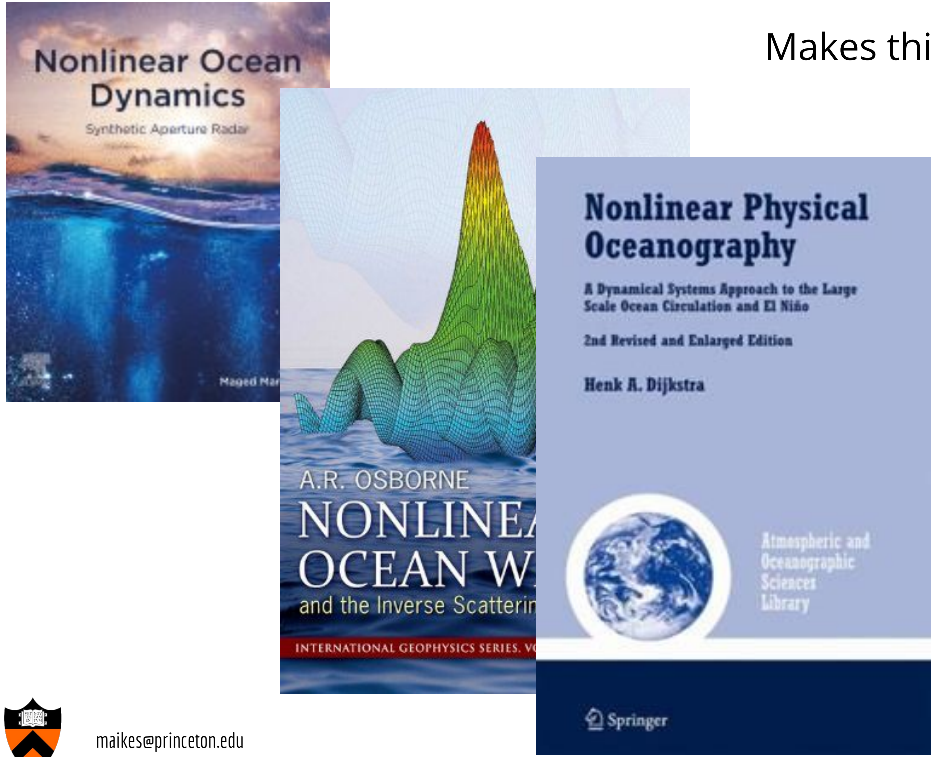
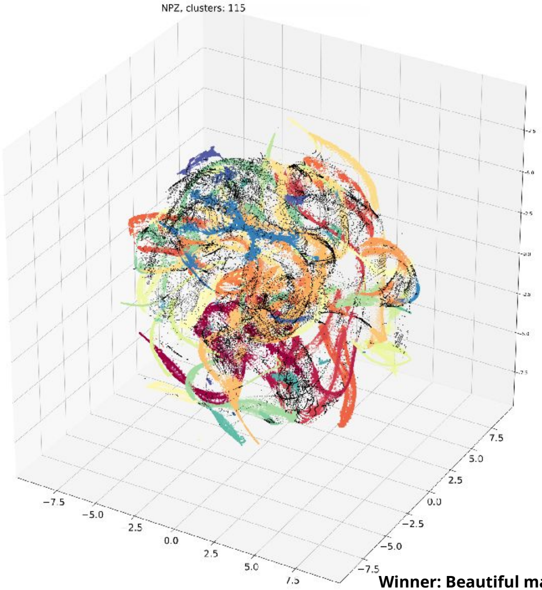
Ocean data need not have a normal distribution



Makes things more difficult, but can be a good thing



Winner: Beautiful math for Simon's foundation

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Useful for non-linear data: t-SNE

We minimize "distance" between lat+lon points in 11D and a low dimensional projection using the Kullbach-Leibner (KL) divergence.

If x_i is the i-th object in 11D, and y_j is the j-th object low-dim space:

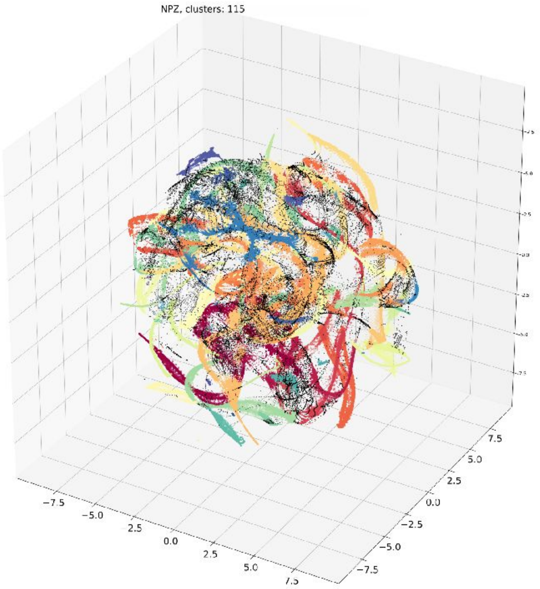
$$p_{j|i} = \frac{\exp(-\mathbf{x}_i - \mathbf{x}_j^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\mathbf{x}_i - \mathbf{x}_k^2/2\sigma_i^2)},$$

and the same for a reduced dimensional set:

$$q_{ij} = \frac{(1+\mathbf{y}_i - \mathbf{y}_j^2)^{-1}}{\sum_{k\neq l}(1+\mathbf{y}_k - \mathbf{y}_l^2)^{-1}}.$$

This is done as:

$$KL(P||Q) = \sum_{i\neq j} p_{ij}\log\frac{p_{ij}}{q_{ij}}$$



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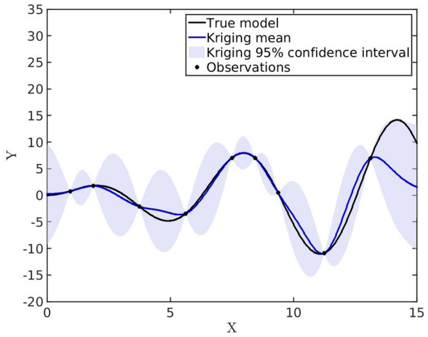
ML in observations: Missing data

- Missing data e.g. having no sample is available for a location
- Popular techniques include Kriging (Gaussian process regression) on satellite fields (Traon et al. 1998)
- Efforts to combine EOF analysis with DL emerging (Barth et al. 2020)
    - Use convolutional neural nets (CNN) and historical data to reconstruct sea surface temperature from satellites.



Lataniotis et al., 2015

Interpolation based on Gaussian process governed by prior covariances

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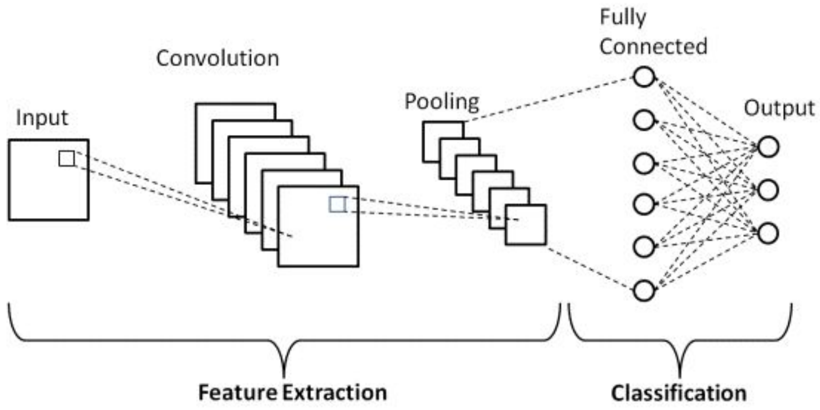
Convolutional Neural Networks (CNN)

CNN benefit:

- Takes local data into account: Can learn lines
- Not fully connected, just aware of sub-area spanned by previous layer
- After `flattening' it goes to a NN



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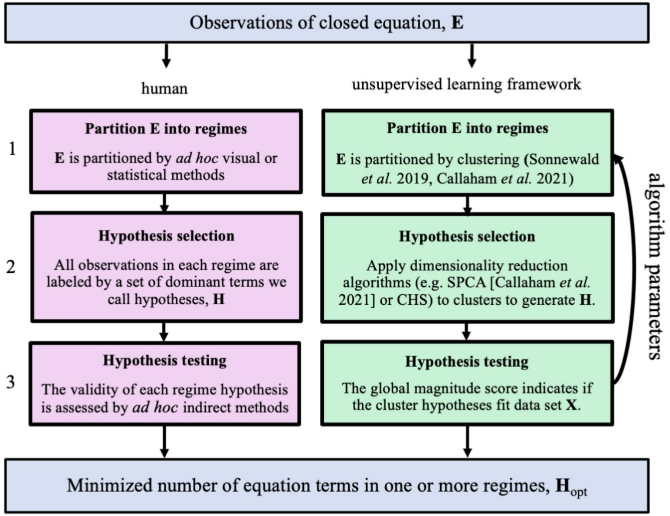
ML and theory

- Theoretical progress is often driven by intuition, and *ad hoc* definition of dynamical regimes
- A dynamical regime constitute local dominant balances between terms, and the boundaries of the solution space in which they are a justifiable truncation of the full dynamics
- ML has been used to remove the ad hoc component offering an unbiased definition of regimes

- `Regime problem' formally defined in Kaiser et al. 2021
- Regimes identified in global circulation (Sonnewald et al. 2019), and in Gulf of Mexico region (Callaham et al. 2020)

Topic of tutorial today



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ML and ocean models: Discretization

- Largely typical fluid following Navier-Stokes
- Discretization necessary, but filamentation results in scale interaction
    - Parameterization of sub-gridscale physics necessary
- Physics-based parameterisations to date do not describe missing physics
- ML is being used to create parameterisation:
    - Direct learning using NN (Bolton and Zanna, 2019)
    - Learning on underlying equation terms with an RVM (Zanna and Bolton, 2020)

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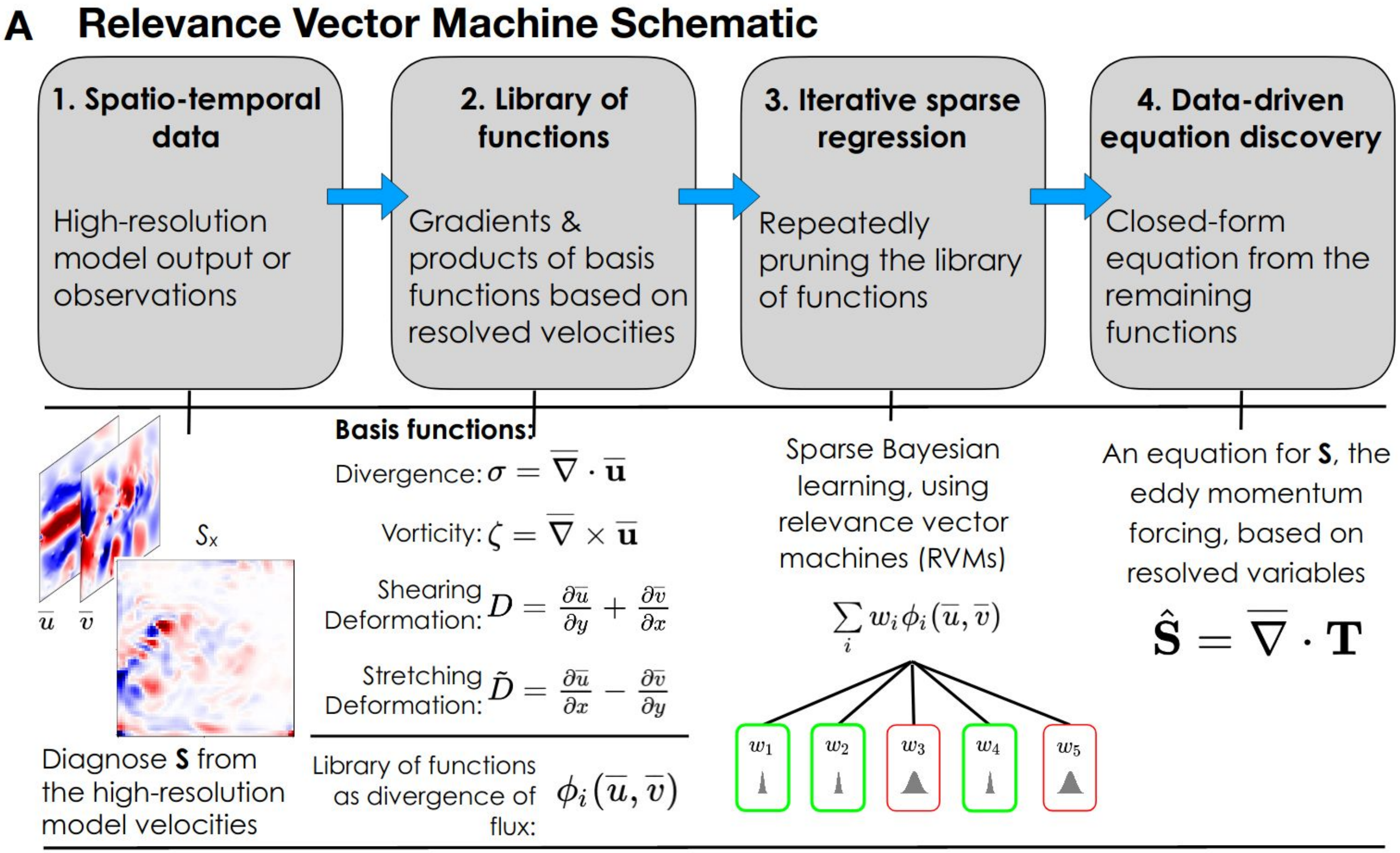

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Zanna and Bolton, 2020

ML and ocean models: Computational challenges

- Improve computational challenges
- ML is a trillion dollar industry based on high performance computing
- Customized hardware (e.g GPUs) is heterogeneous
  - Processing and movement can happen simultaneously
- Move to lower precision (Tinto Prims et al., 2019)
  - Issues with rounding errors due to long timescales in the ocean
- Data centric workflow
  - Remove need for intense input/output with more targeted extraction of data of interest

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ML and predictions: Model bias and error

- Predictions of the ocean (and Earth) system are important to improve
  - Form basis of decision making
- Models can be tested against `truth' benchmark from in-situ or target model data
- Testing and post-processing can also be done `down-scaling', currently largely used within weather prediction
- Bias identification is recently also being done with Layerwise Relevance Propagation (discussed in part 2)

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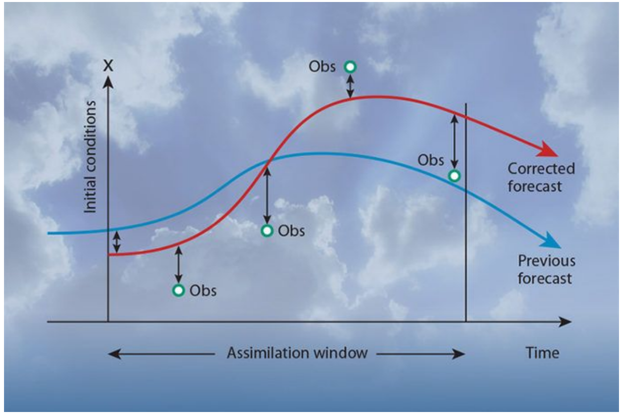
ML and predictions: Data Assimilation



- Tackles initial value problem
- Main forms:
  - Ensemble Kalman filter (EnFK)
  - Four dimensional variational assimilation (4DVar)
- 4DVar has direct ML connection
  - Gradient based cost function minimization
  - Adjoint seen as gradient backpropagation process(Hsieh and Tang, 1998, Kovachki and Stuart, 2019)
- Emulation could be done directly with ML (Brajard et al., 2019, 2020, 2021)
- ML used to pre-process data for assimilation

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ML and decision support

- The case for transparent ML for ocean and climate applications
  - Interpretable AI (IAI) , where model is designed for interpretability (e.g. Rudin, 2019)
  - Explainable AI (XAI), where skill is retrospectively inferred (next lecture)
- `Physics informed' ML: Incorporate theoretical knowledge
  - Embed NN in quasi-geostrophic model (Lguensat et al. 2019)
- ML to provide accurate and actionable information
  - Quantification of uncertainty can be assisted with ML (Schuhen et al., 2012)
- Inform where information is representative
  - Data for Marine Protected areas (Kavenaugh et al., 2016, Sonnewald et al., 2020)

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Summary part 1

- The ocean is an important part of the climate system acting on long timescales
- Recently, large amounts of data have been available, but remaining issues of sparsity
- ML already plays a large role in oceanographic work, within observations, theory, modeling and prediction
- The role of ML will likely increase, with increased emphasis on interpretable and explainable applications

Feel free to start exploring tutorial:
https://github.com/maikejulie/SIAM_ML4Ocean

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Extra

Popular supervised methods

Linear univariate (or multivariate) regression(LR), where the output is a linear combinationof some explanatory input variables. LR is one ofthe first ML algorithms to be studied extensivelyand used for its ease of optimization and its simplestatistical properties [182].

•k-Nearest Neighbors (KNN), where we consider aninput vector, find itskclosest points with regardto a specified metric, then classify it by a pluralityvote of thesekpoints. For regression, we usuallytake the average of the values of thekneighbors.KNN is also known as “analog methods” in thenumerical weather prediction community [164].

•Support Vector Machines (SVM)[62], where theclassification is done by finding a linear separatinghyperplane with the maximal margin between twoclasses (the term “margin” here denotes the spacebetween the hyperplane and the nearest pointsin either class.) In case of data which cannotbe separated linearly, the use of thekernel trickprojects the data into a higher dimension wherethe linear separation can be done.Support VectorRegression (SVR)are an adaption of SVMs forregression problems.

•Random Forests (RF)t hat are a composition of a multitude of Decision Trees (DT). DTs are constructed as a tree-like composition of simple decision rules [29].

•Gaussian Process Regression (GPR)[266], alsocalled kriging, is a general form of the optimalinterpolation algorithm, which has been used inthe oceanographic community for a number ofyears•Neural Networks (NN), a powerful class of uni-versal approximators that are based on composi-tions of interconnected nodes applying geometrictransformations (called affine transformations) toinputs and a nonlinearity function called an “ac-tivation function” [67]: **emulating problems thanks to their built-in uncertainty quantification.**

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Extra

Popular supervised ‘deep learning’ methods

•Multilayer Perceptrons (MLP): when used with-out qualification, this term refers to fully con-nected feed forward multilayered neural networks.They are composed of an input layer that takes theinput data, multiple hidden layers that convey theinformation in a ”feed forward” way (i.e. from in-put to output with no exchange backwards), andfinally an output layer that yields the predictions.Any neuron in a MLP is connected to all the neu-rons in the previous and to those of next layer,thus the use of the term ”fully connected”. MLPsare mostly used for tabular data.

•Convolutional Neural Networks (ConvNet): con-trarily to MLPs, ConvNets are designed to takeinto account the local structure of particular typeof data such as text in 1D, images in 2D, volu-metric images in 3D, and also hyperspectral datasuch as that used in remote sensing. Inspired bythe animal visual cortex, neurons in ConvNets arenot fully connected, instead they receive informa-tion from a subarea spanned by the previous layercalled the ”receptive field”. In general, a ConvNetis a feed forward architecture composed of a se-ries of convolutional layers and pooling layers andmight also be combined with MLPs. A convolu-tion is the application of a filter to an input thatresults in an activation. One convolutional layerconsist of a group of ”filters” that perform mathe-matical discrete convolution operations, the resultof these convolutions are called ”feature maps”.The filters along with biases are the parameters ofthe ConvNet that are learned through backpropa-gation and stochastic gradient descent. Poolinglayers serve to reduce the resolution of featuremaps which lead to compressing the informationand speeding up the training of the ConvNet, theyalso help the ConvNet become invariant to smallshift in input images [156]. ConvNets benefitedmuch from the advancements in GPU computingand showed great success in the computer visioncommunity.

•Recurrent Neural Networks (RNN): with anaim to model sequential data such as temporalsignals or text data, RNNs were developed witha hidden state that stores information aboutthe history of the sequences presented to itsinputs.While theoretically attractive, RNNswere practically found to be hard to train dueto the exploding/vanishing gradient problems,i.e.backpropagated gradients tend to eitherincrease too much or shrink too much at each timestep[128].Long Short Term Memory (LSTM)architecture provided a solution to this problemthrough the use of special hidden units [221].LSTMs are to date the most popular RNNarchitectures and are used in several applicationssuch as translation, text generation, time seriesforecasting, etc.Note that a variant forspatiotemporal data was developed to integratethe use of convolutional layers, this is calledConvLSTM [226]

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Extra

Unsupervised learning

Methods largely in use are for clustering, based on probabilistic methods.

:•k-means, a popular and simple space-partitioningclustering algorithm that finds classes in adataset by minimizing within-cluster variances[232]. Gaussian Mixture Models (GMMs) can beseen as a generalization of the k-means algorithmthat assumes the data can be represented by amixture (i.e. linear combination) of a number ofmulti-dimensional Gaussian distributions [177].

•Kohonen maps [also calledSelf Organizing Maps(SOM)] is a NN based clustering algorithm thatleverages topology of the data; nearby locations ina learned map are placed in the same class [148].K-means can be seen as a special case of SOMwith no information about the neighborhood ofclusters.

•t-SNEandUMAPare two other clusteringalgorithms which are often used for not onlyfinding clusters but also because of their datavisualization properties which enables a twoor three dimensional graphical rendition of thedata [252, 176]. These methods are useful forrepresenting the structure of a high-dimensionaldataset in a small number of dimensions thatcan be plotted. For the projection, they use ameasure of the “distance” or “metric” betweenpoints, which is a sub-field of mathematics wheremethods are increasingly implemented for t-SNEor UMAP.

•Principal Component Analysis(PCA) [192], thesimplest and most popular dimensionality reduc-tion algorithm. Another term for PCA is Empir-ical Orthogonal Function analysis (EOF), whichhas been used by physical oceanographers formany years, also called Proper Orthogonal De-composition (POD) in computational fluids liter-ature.

•Autoencoders(AE) are NN-based dimensionalityreduction algorithms, consisting of a bottleneck-like architecture that learns to reconstruct theinput by minimzing the error between the outputand the input (i.e.ideally the data given asinput and output of the autoencoder should beinterchangeable). A central layer with a lowerdimension than the original inputs’ dimensionis called a “code” and represents a compressedrepresentation of the input [150].

•Generative modeling: a powerful paradigm thatlearns the latent features and distributions ofa dataset and then proceeds to generate newsamples that are plausible enough to belong to theinitial dataset. Variational Auto-encoders (VAEs)and Generative Adversarial Networks (GANS) aretwo popular techniques of generative modelingthat benefited much from the DL revolution [145,112]

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Part 2: Dynamical regime discovery and interpretable/explainable ML

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The dynamical regime problem

- Understanding complex system dynamics advances enabled by finding locally dominant system behaviour: Dynamical regimes
    - Examples: ocean, climate, tumors, turbulent flows, epilepsy, general relativity…
- Many dynamical systems like the ocean have uncomputably large numbers of degrees of freedom
- Within the governing equations, some dynamics of mean variables can be approximately reducible
    - Locally describable by a dominant balance of terms within the governing equations (Callaham et al., 2021)
- A `dynamical regime' are the balances and their boundaries within solution space where they are a reasonable truncation
- Most practical applications have non-asymptotic balances: no parameter permits formal expansion

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Finding dynamical regimes

- Conventional:
    - Forming hypotheses has relied on ad-hoc research or expert intuition
    - Not objective: Subject to human bias
- ML assisted:
    - Offers less biased approach, able to handle large amounts of data
- Formally defined as an optimization problem in Kaiser et al. 2021: *'Objective discovery of dominant dynamical processes with machine learning'*

Examples of Interpretable AI (IAI)
(Rudin 2019, Irrgang et al. 2021, Sonnewald et al. 2021ab)

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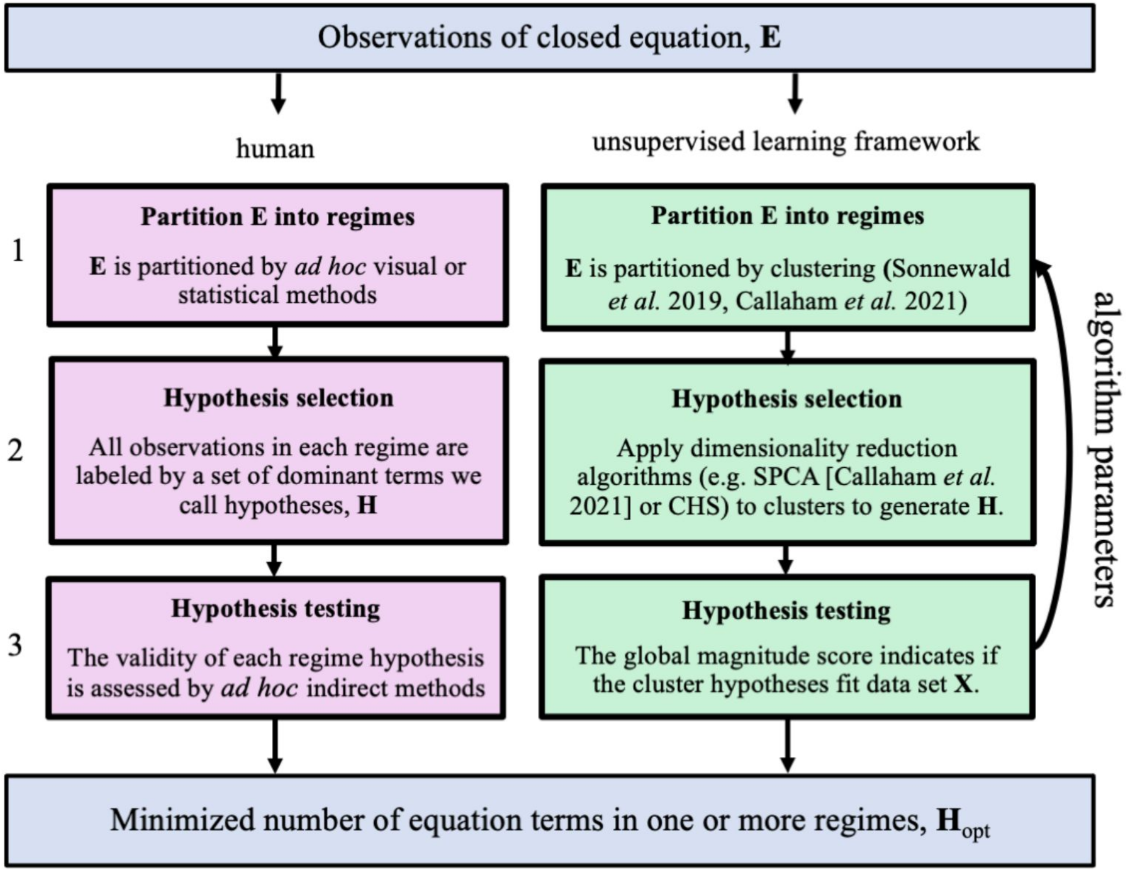

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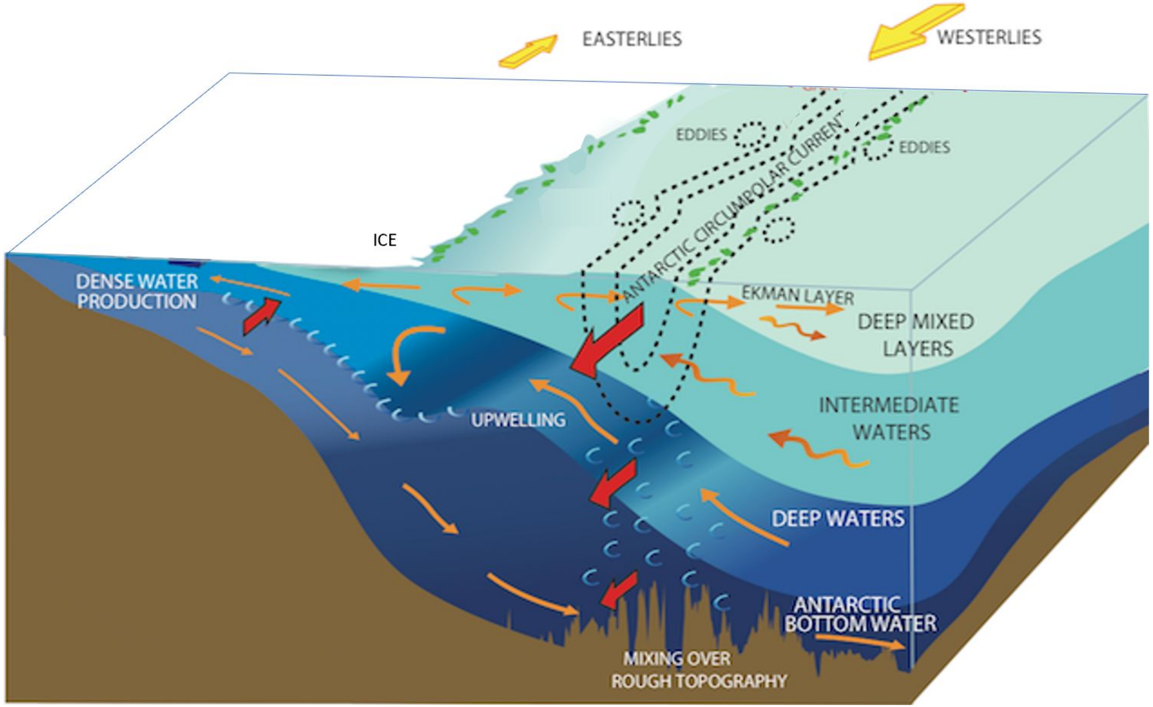
Kaiser et al. 2021

Dynamical regimes in the ocean: What fundamentally controls the circulation?

Are there coherent regions?

Regimes of forcings on the ocean?

Can be used to:
- Predict changes
- Develop better models
- Fundamental understanding



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Equation space transformation

Momentum eqs.

$$\partial_t \mathrm{u} + f\mathrm{k}\times\mathrm{u} = -\frac{1}{\rho_0}\nabla_h \mathrm{p} + \frac{1}{\rho_0}\partial_z \tau + \mathrm{a} + \mathrm{b}, \partial_z \mathrm{p} = -\mathrm{g}\rho$$

$$\nabla_h \cdot \mathrm{u} + \partial_z w = 0,$$

Depth integrate, take curl

$$\overbrace{\nabla\cdot(f\mathbf{U})}^{\text{advection of planetary vorticity}} = \frac{\overbrace{\nabla p_b \times \nabla H}^{\text{bottom pressure torque}}}{\rho} + \frac{\overbrace{\nabla\times\boldsymbol{\tau}}^{\text{wind \& bottom stress curl}}}{\rho} + \overbrace{\nabla\times\mathbf{A}}^{\text{nonlinear torque}} + \overbrace{\nabla\times\mathbf{B}}^{\text{diffusive torque}}.$$

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Equation space transformation

Primitive equations

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} - fv = -\frac{1}{\rho_o}\frac{\partial P}{\partial x} + \frac{\partial}{\partial z}\left(K_m\frac{\partial u}{\partial z}\right) + F_u, \quad \text{Momentum (u component)}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} + fu = -\frac{1}{\rho_o}\frac{\partial P}{\partial y} + \frac{\partial}{\partial z}\left(K_m\frac{\partial v}{\partial z}\right) + F_v \quad \text{Momentum (v component)}$$

$$\frac{\partial P}{\partial z} = -\rho g, \quad \text{density}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \quad \text{continuity}$$

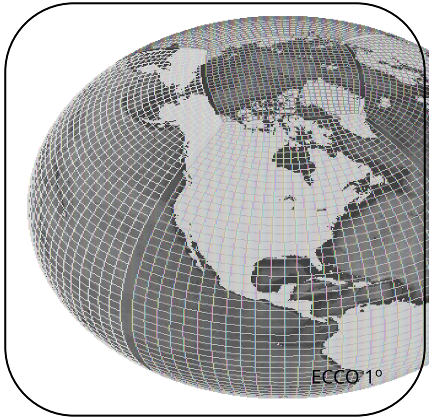
$$\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} + w\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z}\left(K_h\frac{\partial \theta}{\partial z}\right) + F_\theta, \quad \text{Advection of temperature}$$

$$\frac{\partial s}{\partial t} + u\frac{\partial s}{\partial x} + v\frac{\partial s}{\partial y} + w\frac{\partial s}{\partial z} = \frac{\partial}{\partial z}\left(K_h\frac{\partial s}{\partial z}\right) + F_s, \quad \text{Advection of salinity}$$

$$\rho = \rho(\theta, s), \quad \text{Density as a function of S and T}$$

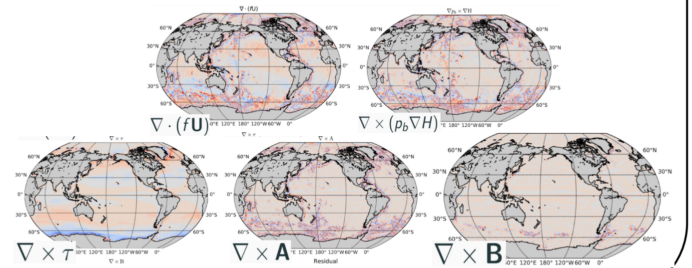
Ocean model that follows laws of physics

Huge number of 3D fields



Use theory to reduce dimensions and enhance interpretability

$$0 = \overbrace{\nabla \cdot (f\mathbf{U})}^{\text{Advection}} - \underbrace{\nabla \times (p_b \nabla H)}_{\text{Bottom Pressure Torque}} + \overbrace{\nabla \times \tau}^{\text{Wind and Bottom stress}} - \underbrace{\nabla \times \mathbf{A}}_{\text{Non-linear Torque}} + \overbrace{\nabla \times \mathbf{B}}^{\text{Lat. Visc.}}$$



Arrive at five 2D fields:
- Each term in the equation

Ask: Are there patterns?

Example from Sonnewald et al. 2019

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Dynamical regimes in the ocean

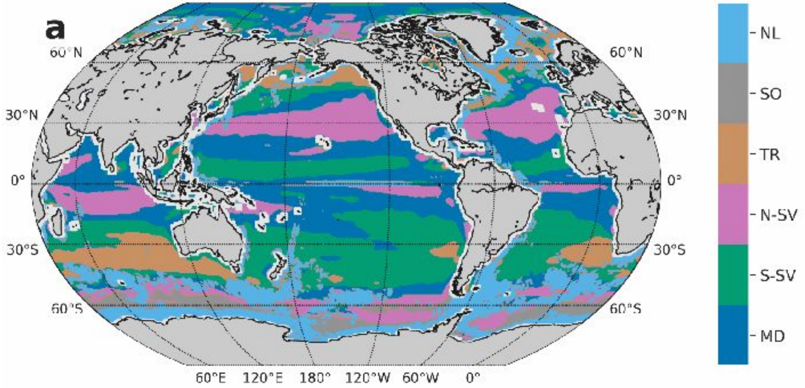
NOAA Artificial Intelligence Strategy
Analytics for Next-Generation Earth Science

Apply clustering

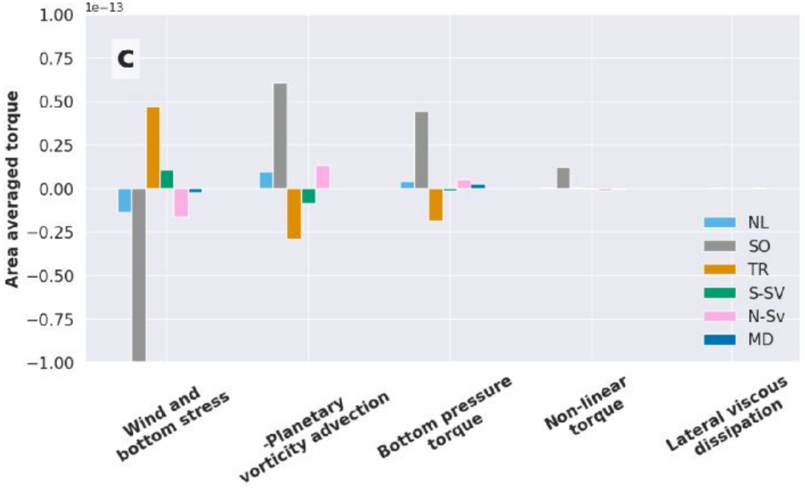
$$J = \sum_{j=1}^{k} \sum_{i=1}^{n} \overbrace{||x_i^j - c_j||^2}^{\text{Distance function}}$$

cluster guess: k; data: n; data point: x_i^j; centroids: c_j

Rigorous model selection tests



Clustering generates a set of hypotheses regarding the groupings of the data:



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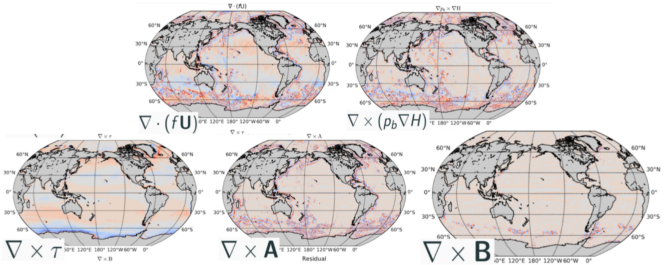
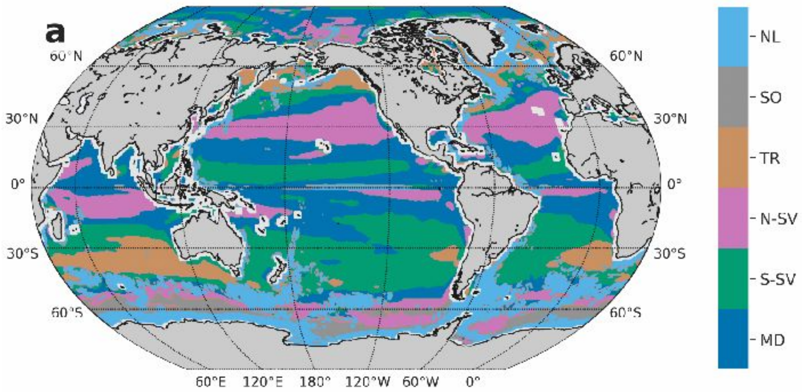
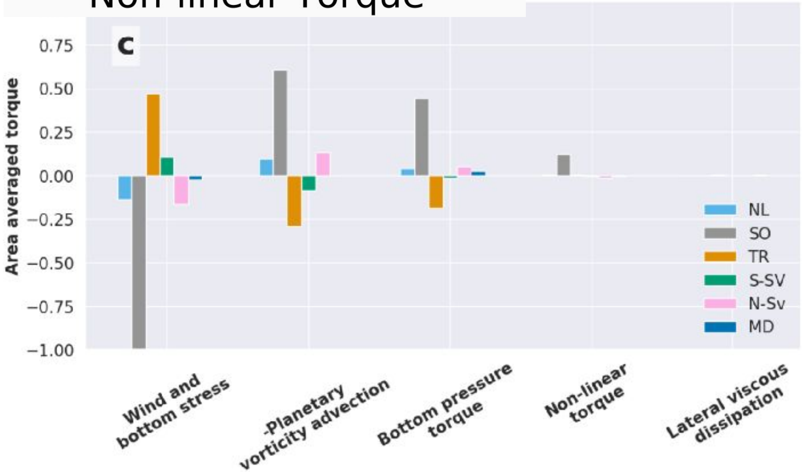


model

Clustering generates a set of

$$0 = \overbrace{\nabla \cdot (f\mathbf{U})}^{\text{Advection}} - \underbrace{\nabla \times (p_b \nabla H)}_{\text{Bottom Pressure Torque}} + \overbrace{\nabla \times \tau}^{\text{Wind and Bottom stress}} - \underbrace{\nabla \times \mathbf{A}}_{\text{Non-linear Torque}} + \overbrace{\nabla \times \mathbf{B}}^{\text{Lat. Visc.}}$$





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Practical: Arriving at hypotheses with ML

https://github.com/AOS551/MLINT

launch binder

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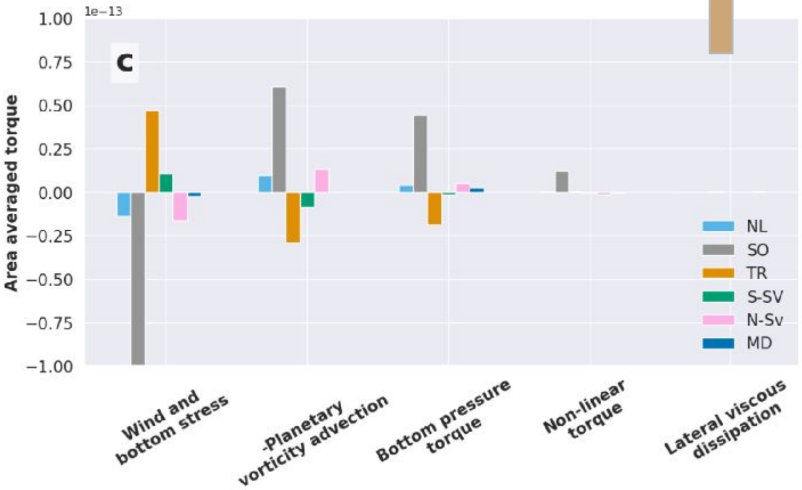
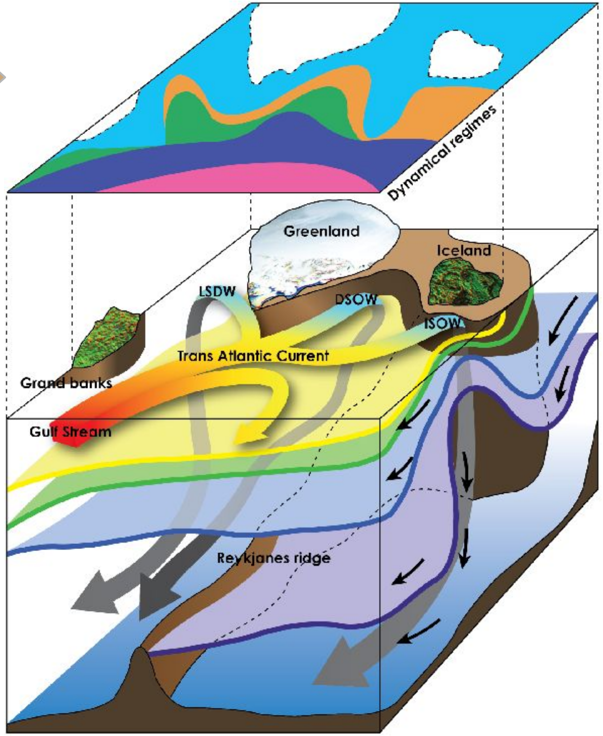
Practical: Arriving at hypotheses with ML



Map neatly onto circulation crucial to climate



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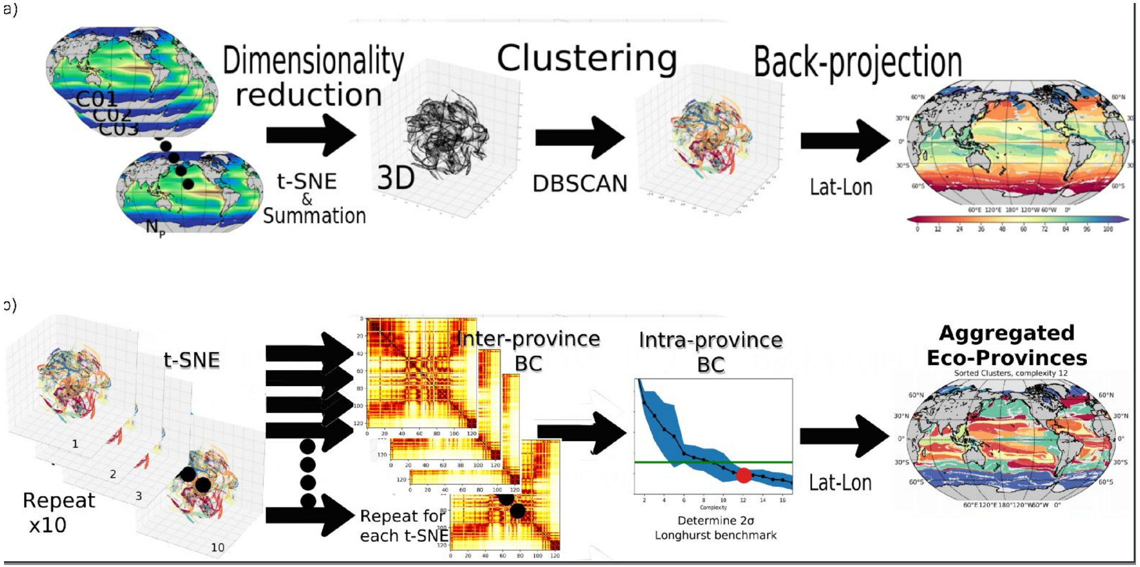
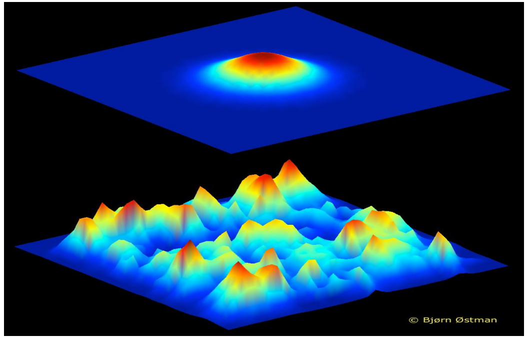
More complex optimization problems



- Highly non-gaussian
- Resort to more stochastic methods
- Visualization to guide clustering
- Complicated optimization space
- Combination of domain knowledge and graphs to arrive at robust results



Systematic AGgregated Ecoprovince (SAGE) method
Ocean ecology example (Sonnewald et al. 2020):

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Useful projection methods: t-SNE

We minimize "distance" between lat+lon points in 11D and a low dimensional projection using the Kullbach-Leibner (KL) divergence.

If x_i is the i-th object in 11D, and y_j is the j-th object low-dim space:

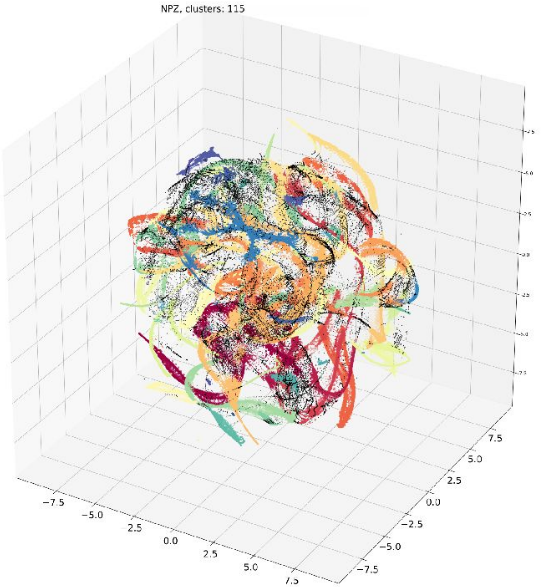
$$p_{j|i} = \frac{\exp(-\mathbf{x}_i - \mathbf{x}_j^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\mathbf{x}_i - \mathbf{x}_k^2/2\sigma_i^2)},$$

and the same for a reduced dimensional set:

$$q_{ij} = \frac{(1+\mathbf{y}_i - \mathbf{y}_j^2)^{-1}}{\sum_{k\neq l}(1+\mathbf{y}_k - \mathbf{y}_l^2)^{-1}}.$$

This is done as:

$$KL(P||Q) = \sum_{i\neq j} p_{ij}\log\frac{p_{ij}}{q_{ij}}$$



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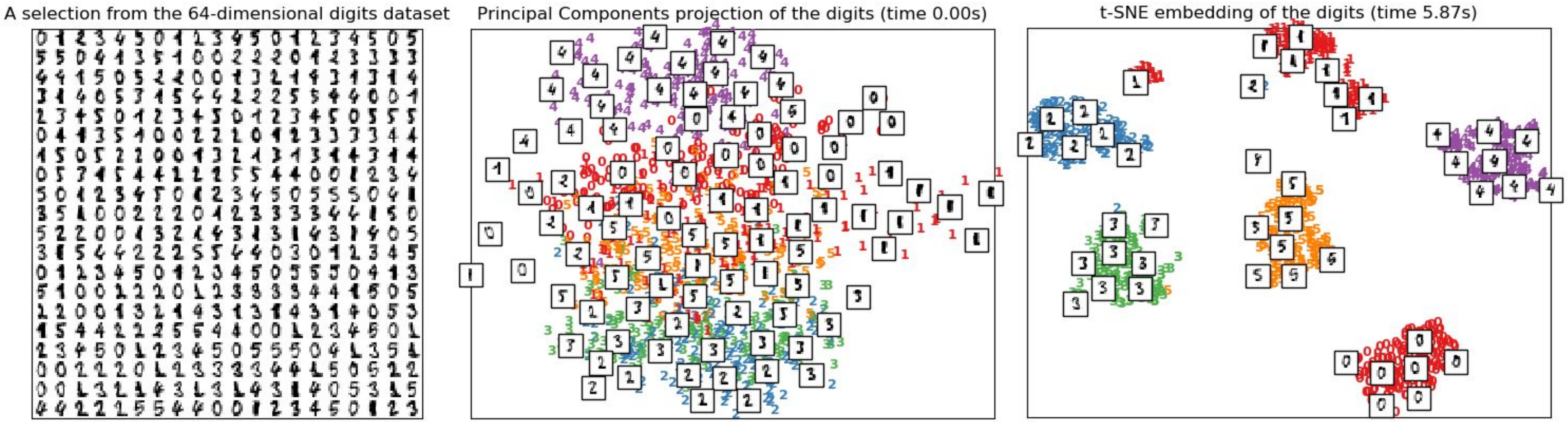
Principal Component Analysis vs. t-SNE



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Explainable AI (XAI):
Learning how the NN achieves predictive skill

- Set of popular `Additive Feature Attribution’ methods:
    - Local Interpretable Model-agnostic Explanations (LIME)
    - Layer-wise Relevance Propagation (LRP)
    - Shapley Additive Explanation (SHAP)
- Other methods based on saliency

- Class of highly sought after methods

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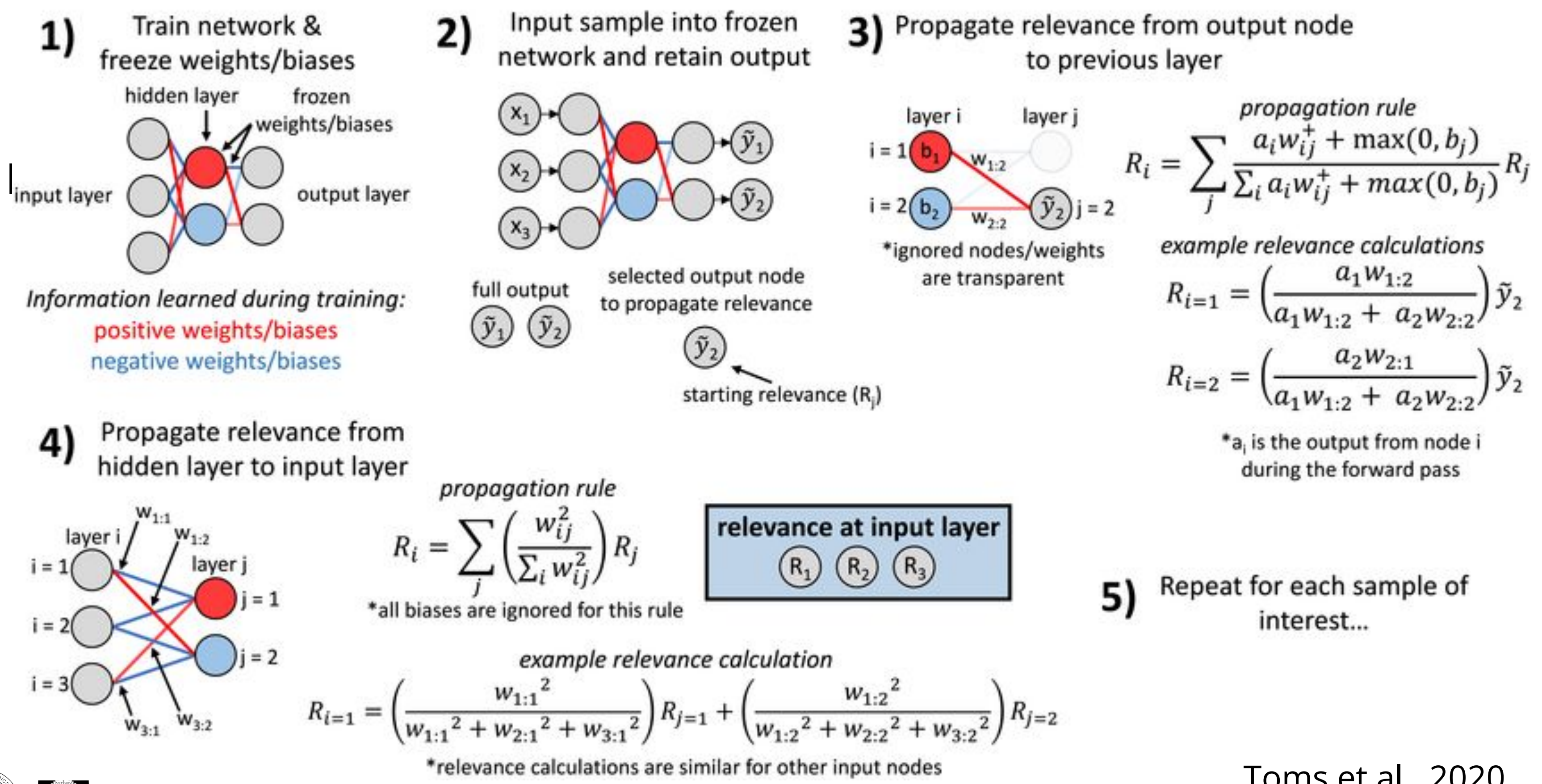
Illustration of Layerwise Relevance Propagation



Toms et al., 2020

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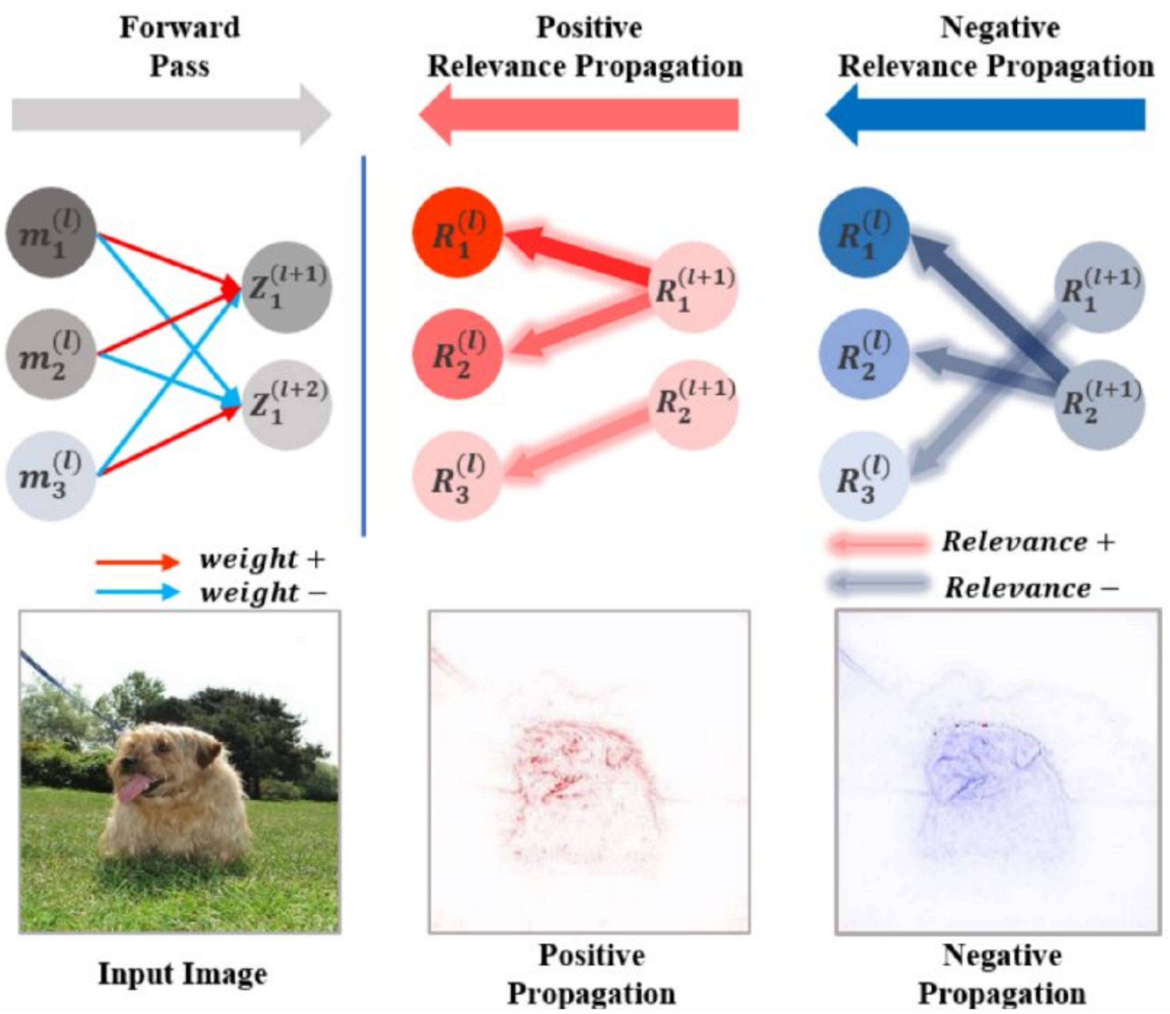
LRP example



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Implications for XAI for oceanography: Case study

- Dynamical recognition/sanity check
- For high-stakes decisions, stepping out of `black box’ is key
- Can help with generalization problem
- Can help avoid underspcification

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Deep Neural Network trained to predict regimes

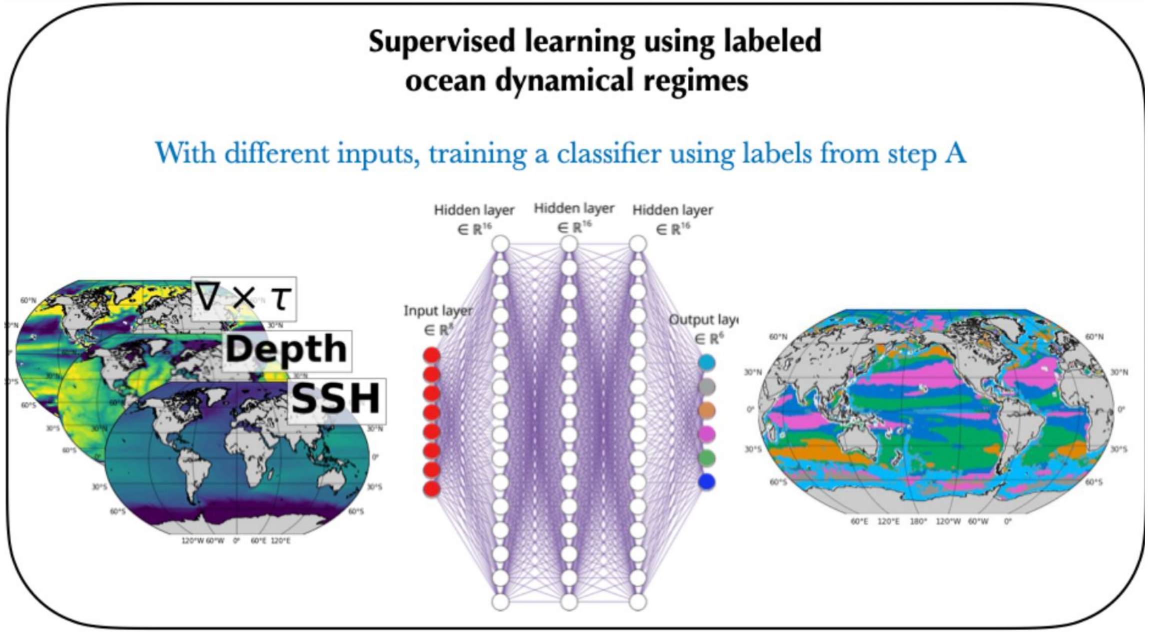
Train Multilayer perceptron using inputs:

- Wind stress
- Sea surface height
- Depth

Predict:

- Dynamical regimes

Developed network can be applied to models where the input variables are available



From Sonnewald and Lguensat, 2021

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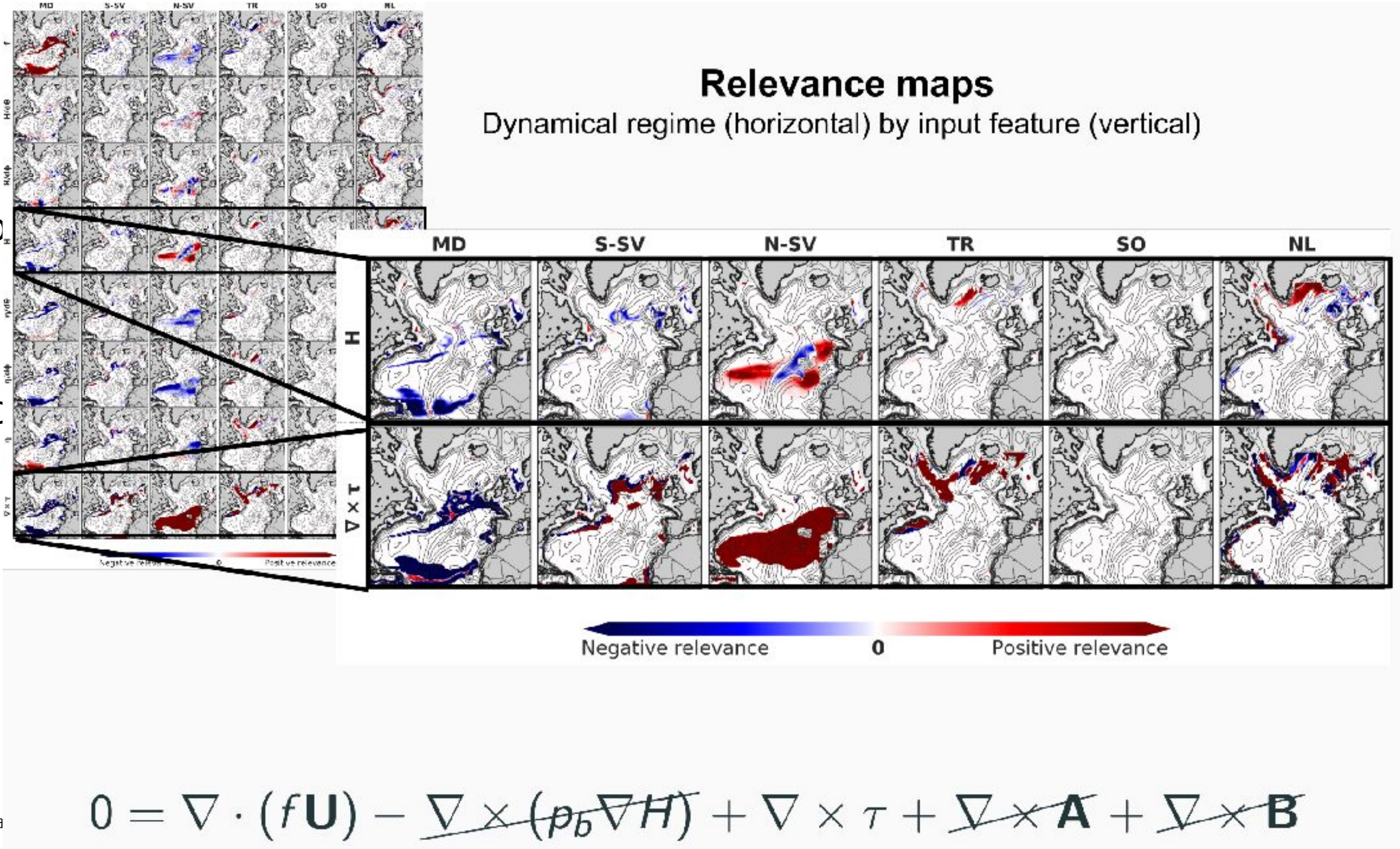

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Using Additive Feature Attribution?

- While not perfect, LRP are useful in predicting ocean dynamical regimes
    - Somewhat circular logic as LRP and MLP are tested simultaneously
- Other methods have drawbacks:
    - LIME assumes sparse linear model can represent relationship to all features
    - SHAP uses possible brittle game theoretic component
- Overall improving AFA methods to better be able to explore the local feature space would be powerful within oceanography and beyond

Example of dynamical regimes with LRP:
https://github.com/maikejulie/DNN4Cli

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Summary part 2

- Dynamical regimes within dynamical systems
- Global ocean dynamical regimes
- Demonstrated how statistical and domain specific criteria are used
- Looked at more complex optimization problems
- Explainable AI: Challenges and opportunities

Review: M. Sonnewald, R. Lguensat, D. Jones, P. Deuben, J. Brajard, V. Balaji: `Bridging observation, theory and numerical simulation of the ocean using ML', Environmental Research Letters. 2021.

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