basic Intro to Machine Learning

Outline

(Just overview here; for actual content see Jupyter notebooks)

- a very loose introduction to Machine Learning (ML)
  $\rightarrow$ as a problem in regression / optimisation
  $\rightarrow$ supervised vs. unsupervised
  $\rightarrow$ sample usage in oceanography

- example with argo data
  $\rightarrow$ what is Argo?
  $\rightarrow$ unsupervised ML example: clustering analysis
  $\rightarrow$ supervised ML example: neural networks

Some propaganda to start with

ML algorithms are:

- algorithms + tools, and that's it

  $\rightarrow$ very powerful, but context dependent

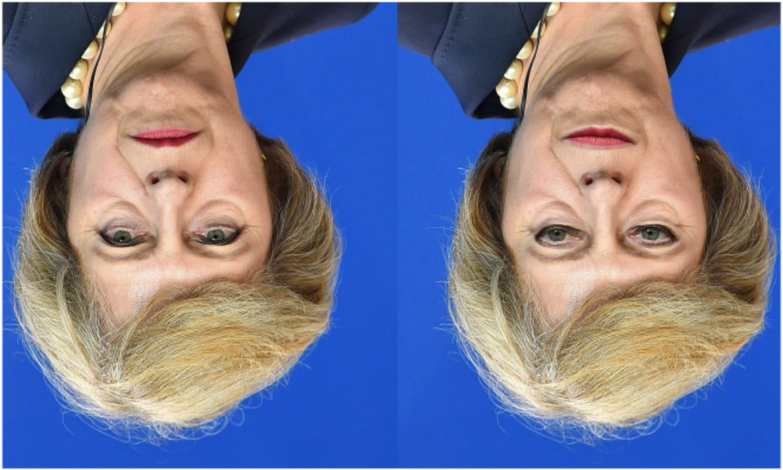
- usually black box

  $\rightarrow$ it can work wonderfully / fail spectacularly, but you don't necessarily know why...

!!! prudent to do sanity checks!

Figure: Hermeowus Mora, disciple of Hermaeus Mora the Daedric prince of knowledge and memory

Cursed example: image recognition/generation



Cursed example: image recognition/generation

Machine learning + regression/optimisation

Recall that, in regression, for X the input, Y the output, f the model, where

$$Y = f(X),$$

the aim is to seek f such that we minimise something like

$$J = \sum_i (Y_i - f(X_i))^2$$

$\rightarrow$ e.g. linear regression, polynomial fitting

- ML in a nutshell follows the same principle

  $\rightarrow$ algorithms are different (e.g. nonlinear, network based, different optimiser, stochastic/probabilistic)

Training, Validation, Testing data

Normally split (X, y) into

- training data $(X_{\text{train}}, Y_{\text{train}})$ (most data should be here)

  $\rightarrow$ exposed to ML algorithms for training the model

  $\rightarrow$ used to compute misfits or loss function

- validation data $(X_{\text{val}}, Y_{\text{val}})$

  $\rightarrow$ exposed to ML algorithms to tune model hyperparameters and/or model selection

- test data $(X_{\text{test}}, Y_{\text{test}})$

  $\rightarrow$ **NOT** exposed to ML algorithm

  $\rightarrow$ used to test performance of model

!!! sometimes "validation" and "test" are swapped

Unsupervised vs. supervised

- unsupervised ML is where data is unlabelled, and algorithm picks out features by themselves
  $\rightarrow$ e.g. PCA (so EOFs), clustering, some examples of neural networks

Figure: Cursed cats/dogs (?) from PCA. Figure adapted from Fig. 10 of Brunton, Brunton, Proctor & Kutz (2013).

Unsupervised vs. supervised

- supervised ML is where data is labelled, and algorithm fits model between input and output

  $\rightarrow$ often want this for prediction purposes

  $\rightarrow$ e.g. (multi-)linear regression, some examples of neural networks

- other characterisations (e.g. semi-supervised, reinforcement)

Unsupervised vs. supervised

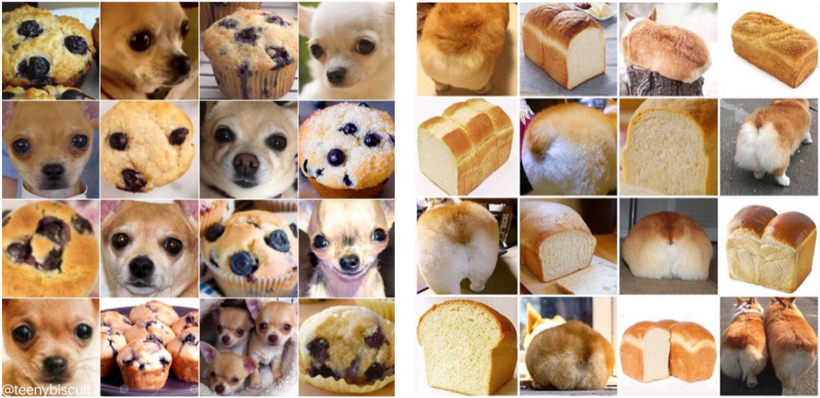


Figure: Various entries from the “animal or things” meme, as found on the internet.

Unsupervised vs. supervised

Figure: Various entries from the "animal or things" meme, as found on the internet.

Oceanographic examples

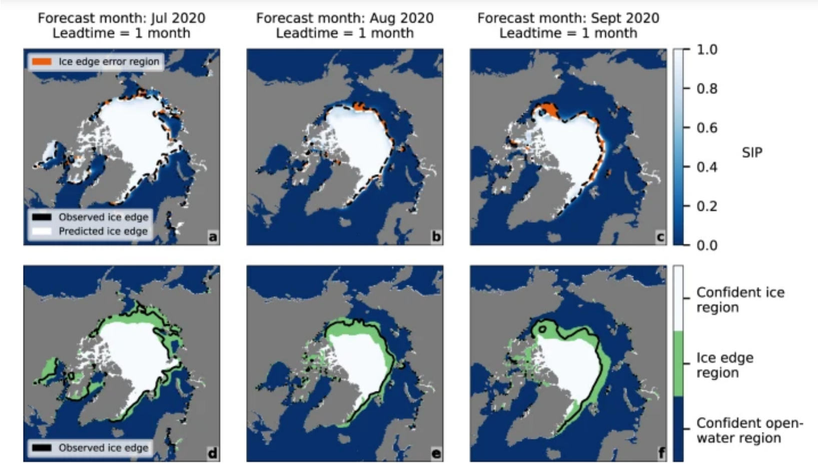


Figure: From Andersson *et al.* (2021), Fig. 7. Convolutional Neural Network to predict sea ice coverage.

Oceanographic examples

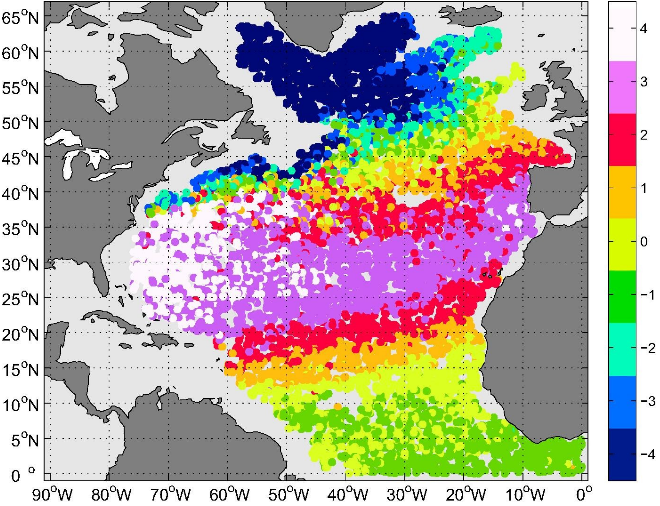


Figure: From Maze *et al.* (2017), Fig. 4. Gaussian Mixture Model to identify watermass clusters from Argo data in Atlantic.

Oceanographic examples

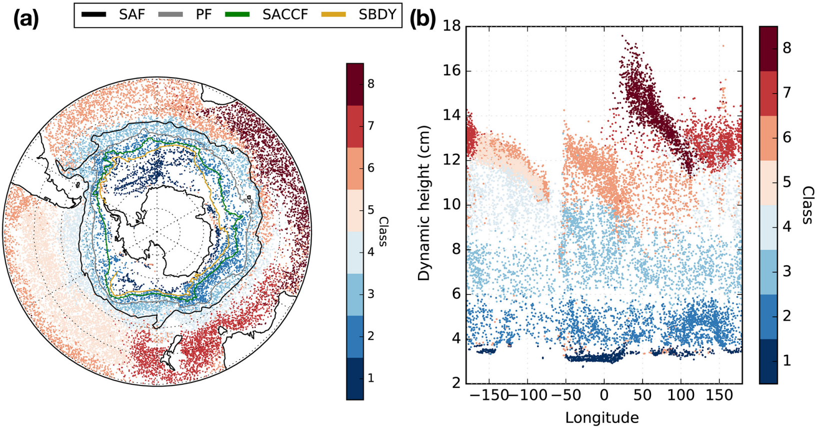


Figure: From Jones *et al.* (2019), Fig. 5. Gaussian Mixture Model to identify watermass clusters from Argo data in Southern Ocean.

Oceanographic examples

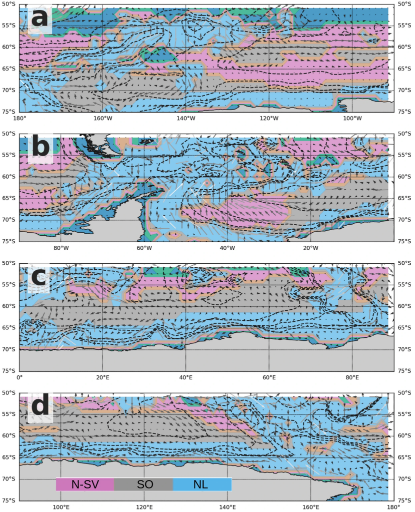


Figure: From Sonnewald *et al.* (2023), Fig. 4. *k*-means to identify clusters based on dynamic (from barotropic vorticity budget).

Oceanographic examples

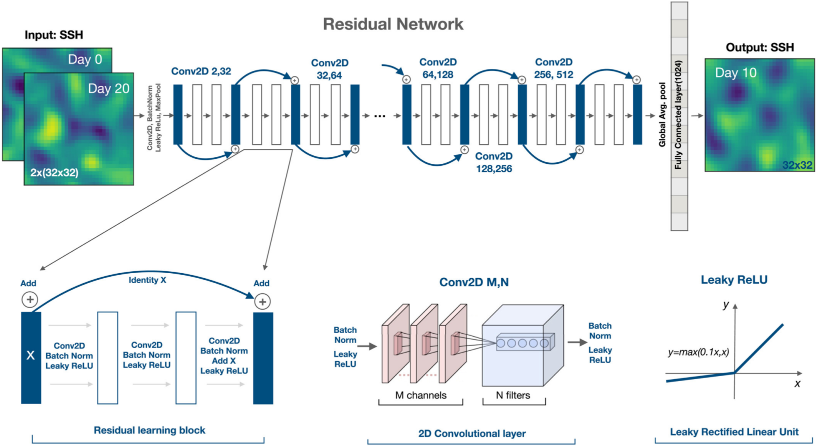


Figure: From Manucharyan *et al.* (2021), Fig. 1. Deep Neural Network to do spatio-temporal interpolation of SSH (with an aim to be dynamically consistent).

Oceanographic examples

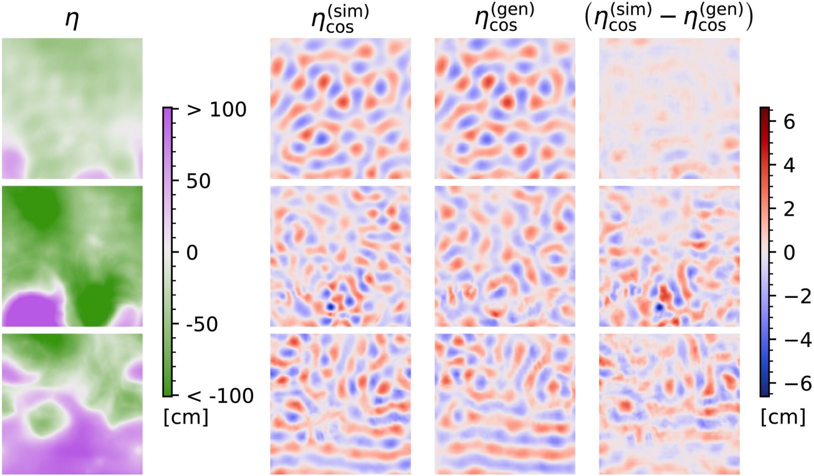


Figure: From Wang *et al.* (2022), Fig. 2. Using a conditional Generative Adversarial Network to extract internal tides from sea surface heigh data.

Oceanographic examples

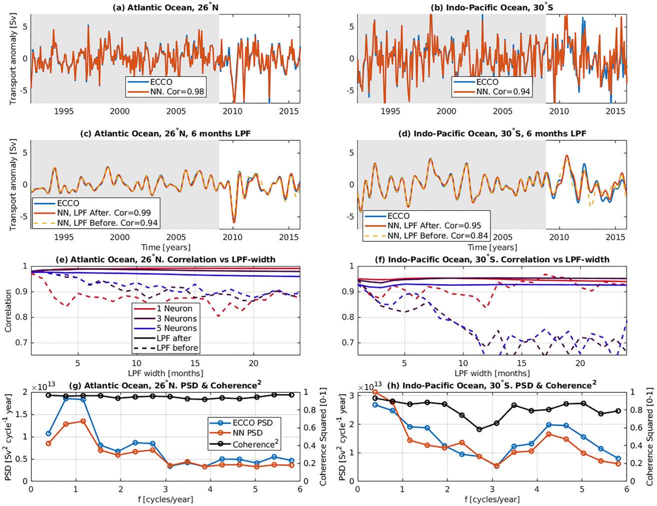


Figure: From Solodoch *et al.* (2023), Fig. 3. Neural Network to AMOC from observables, trained up on a dynamically consistent state estimate.

Oceanographic examples

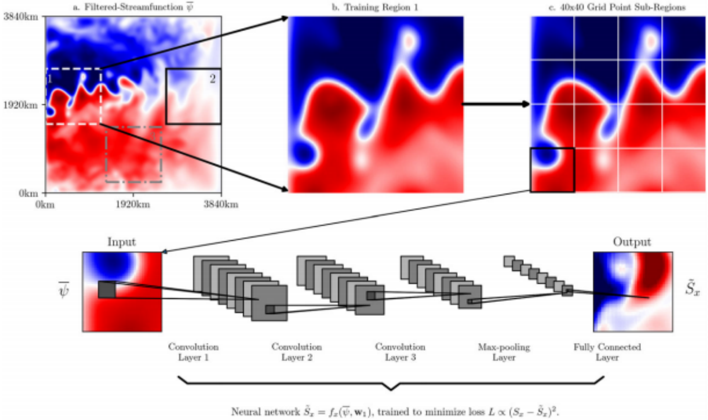


Figure: From Bolton & Zanna (2019), Fig. 1. Convolutional Neural Network for sub-grid parameterisation (regressing eddy fluxes with time-mean streamfunction).

Example: Argo

- A CTD gets
  $\rightarrow$ conductivity to get S
  $\rightarrow$ temperature for T
  $\rightarrow$ it really measures p to get depth
  $\rightarrow$ can put other sensors on (e.g. pH, oxygen, etc.)
- argo system consists of CTDs that floats around the ocean

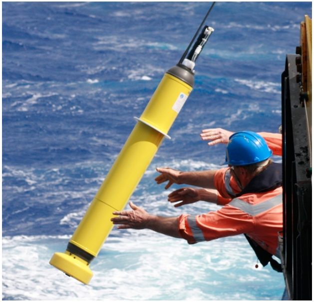


Figure: An Argo float being thrown off a ship. Image from NOAA.

Example: Argo

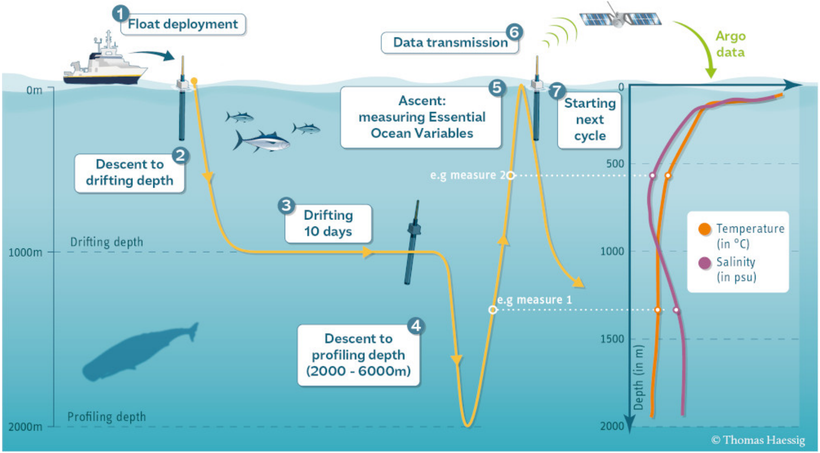


Figure: Argo float cycle schematic. From `argo.ucsd.edu`

Example: Argo

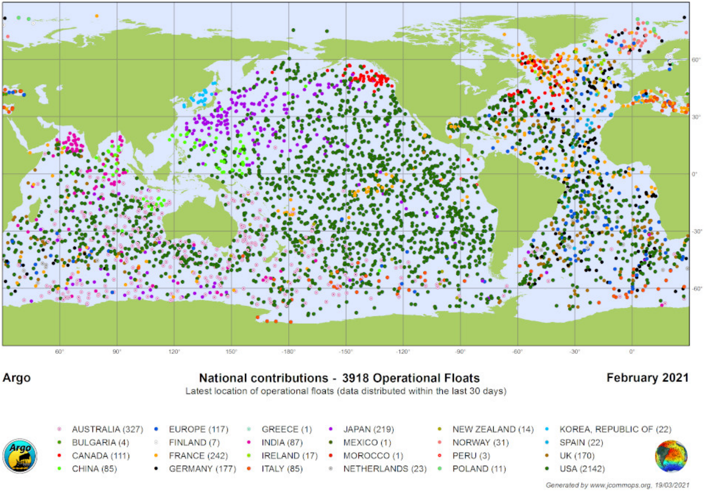


Figure: Argo locations as of Feb 2021. Note the dots are enhanced in size, so coverage is not as dense as it seems. From `argo.ucsd.edu`

Example: Argo

▸ Dimensions: (**DEPTH**: 302, N_PROF: 128910)

▾ Coordinates:

DEPTH	(DEPTH)	float32	0.0 -5.0 -10.0 ... -1500.0 -1505.0
LATITUDE	(N_PROF)	float32	dask.array<chunksize=(67010,), meta=n...
LONGITUDE	(N_PROF)	float32	dask.array<chunksize=(67010,), meta=n...
TIME	(N_PROF)	datetime64[ns]	dask.array<chunksize=(64455,), meta=n...

▾ Data variables:

BRV2	(N_PROF, DEPTH)	float32	dask.array<chunksize=(67010, 302), met...
DBINDEX	(N_PROF)	float64	dask.array<chunksize=(67010,), meta=n...
PSAL	(N_PROF, DEPTH)	float32	dask.array<chunksize=(67010, 302), met...
SIG0	(N_PROF, DEPTH)	float32	dask.array<chunksize=(67010, 302), met...
TEMP	(N_PROF, DEPTH)	float32	dask.array<chunksize=(67010, 302), met...

▸ Attributes: (12)

Figure: Argo dataset in zarr format opened as a xarray object.

- argo data to be downloaded given in zarr format
  → need `zarr` package, can open data through `xarray`
  → ungridded data here
  → see also `argopy` package

Example: Argo

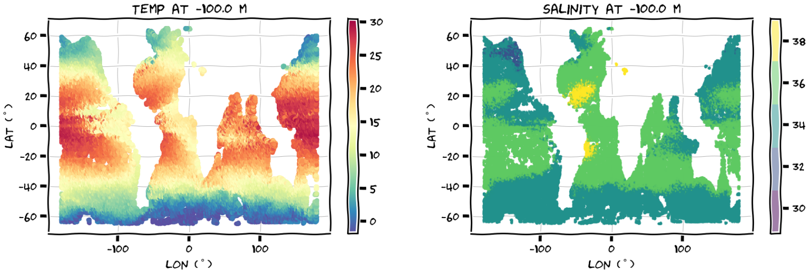


Figure: Argo (in-situ) temperature and (practical) salinity at some fixed depth as a scatter plot coloured by data entry.

- ungridded data, each point is an entry
  $\rightarrow$ scatter plot, with dot coloured by data

Clustering

- we know different watermasses have different properties
  $\rightarrow$ e.g. NADW is more salty
  $\rightarrow$ unsupervised learning?

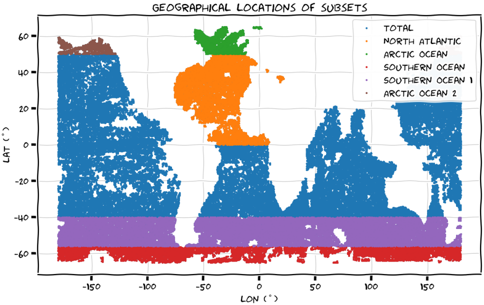


Figure: Artificial clustering.

Clustering

- we know different watermasses have different properties
  → e.g. NADW is more salty
  → unsupervised learning?

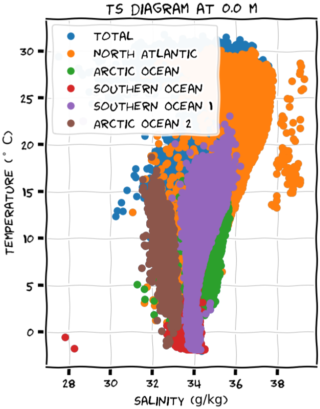


Figure: Artificial clustering as above, but in *TS*-diagram.

Clustering

- one example is *k*-means
  → partition data and find means
  → move partitions slightly and compute new means
  → iterate on partitions such that distance to partition means are minimised (finds local minimums)

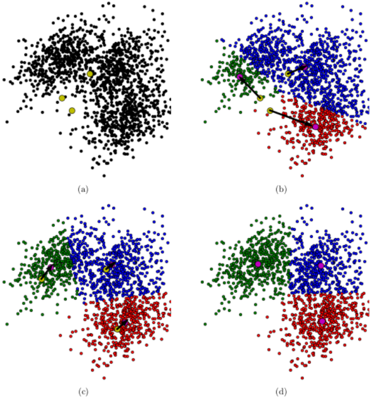
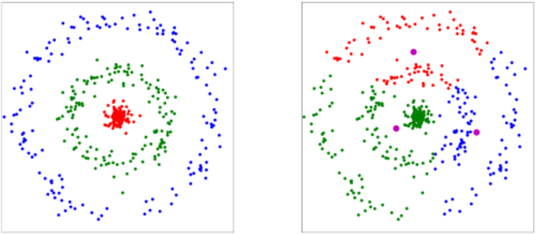


Figure: Demonstration of *k*-means algorithm. Diagram taken from Machine Learning course of Christoph Haase and Varun Kanade at University of Oxford.

Clustering

- example where k-means can fail



(a) Data with three clusters as concentric circles (b) Output of k-means algorithm

Figure: Demonstration of failure of k-means algorithm. Diagram taken from Machine Learning course of Christoph Haase and Varun Kanade at University of Oxford.

Clustering

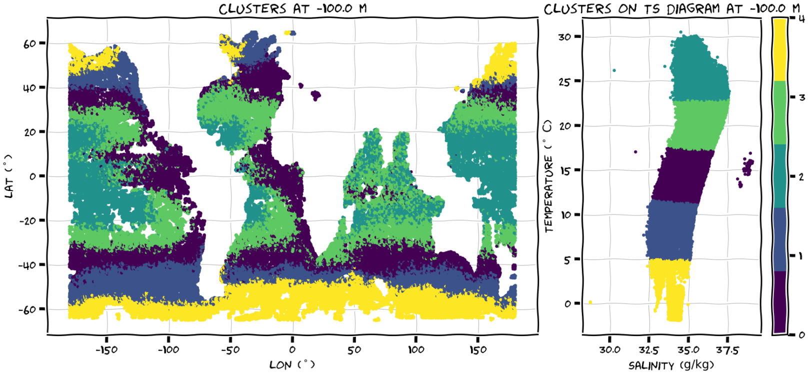


Figure: Clustering from k-means algorithm.

- k-means in TS-space really
- some physical rationalisation possible

!!! didn't standardise data here (probably should have)

Clustering

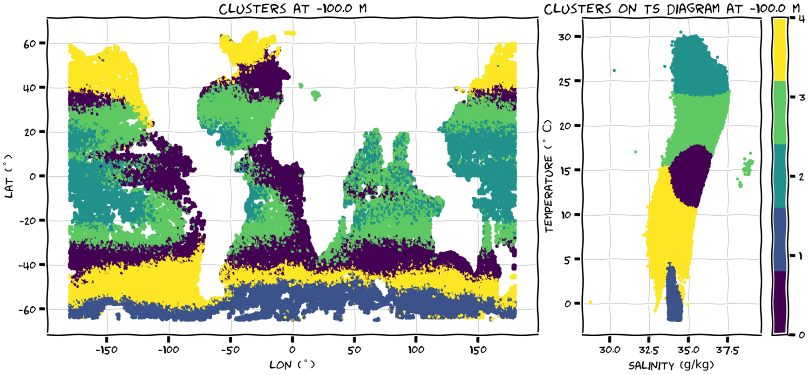


Figure: Clustering from Gaussian Mixture Model.

- similar to above but with some subtle differences
- GMM used in oceanography before (e.g. Jones *et al.*, 2019, in Southern Ocean)

!!! didn't standardise data here (probably should have)

Neural Network

- suppose we want to predict salinity from temperature, i.e. prediction/reconstruction

  → more for demonstration really...

  → split data first (`sklearn.train_test_split`)

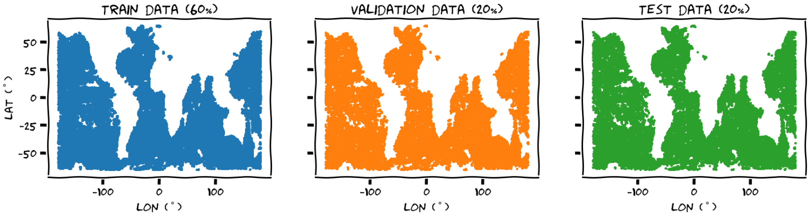


Figure: Splitting of argo data into training:validation:test as 60:20:20.

Neural Network

- linear regression?
  $\rightarrow$ standardise data
  $\rightarrow$ train with training data (could in principle use everything)

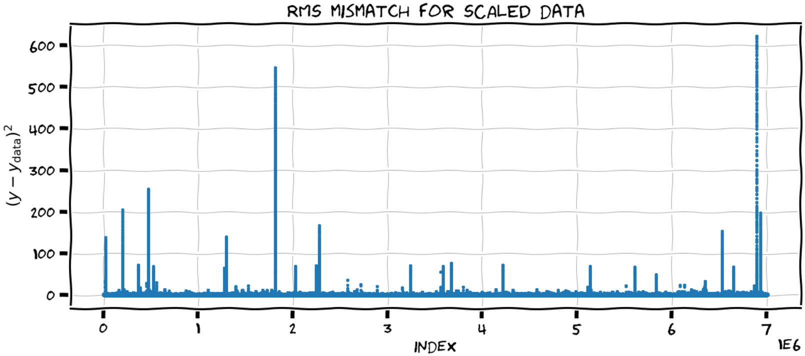
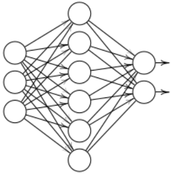
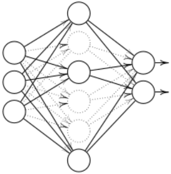


Figure: Root-mean-square loss against index for scaled data, so anything larger than 1 is pretty bad.

Neural Network



(a) Neural Network



(b) Neural Network with Dropout

Figure: Schematic of neural network. Diagram adapted from Machine Learning course of Christoph Haase and Varun Kanade at University of Oxford.

- a neural network has

  → nodes containing features or transformation rules

  → links linking the nodes

  → weights tagged with links specifying weighting or transition probability going from one node to another

- simple case would be adjusting weights to minimise the mismatch / loss function

  → could in principle adjust features in nodes etc.

  → drop off procedure as a stabiliser

Neural Network

- train model with training and validation data
  $\rightarrow$ data has been standardised here
- model trained over 30 epochs
  $\rightarrow$ think 30 complete passes/iterations

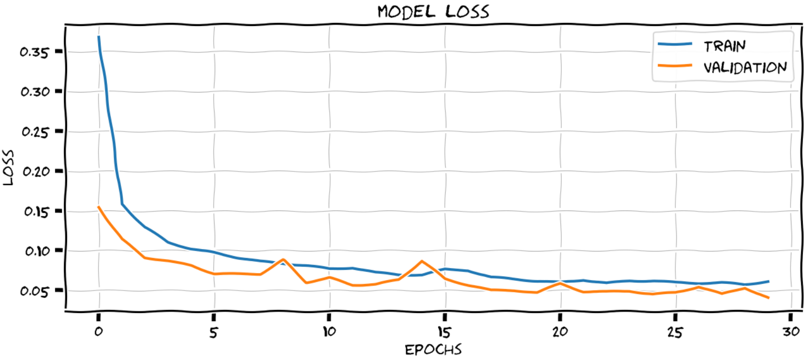


Figure: RMS loss against epoch. Note the RMS loss is not zero (and we don't expect it to be).

Neural Network

- model takes an input depth varying in-situ temperature and returns a salinity profile

  → three random realisations below, with scaling inverted

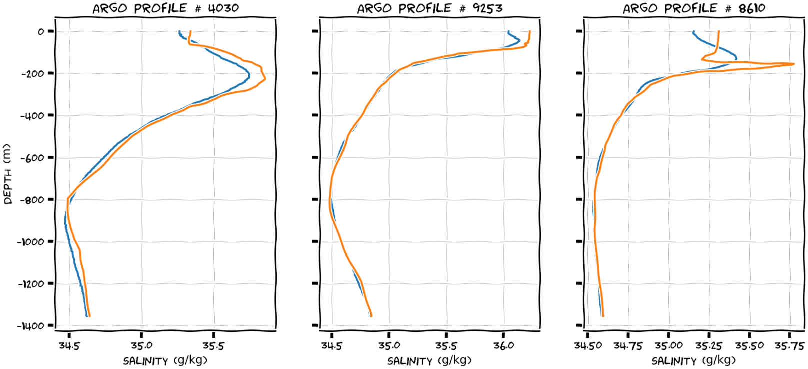


Figure: Three examples of using the trained neural network.

Neural Network

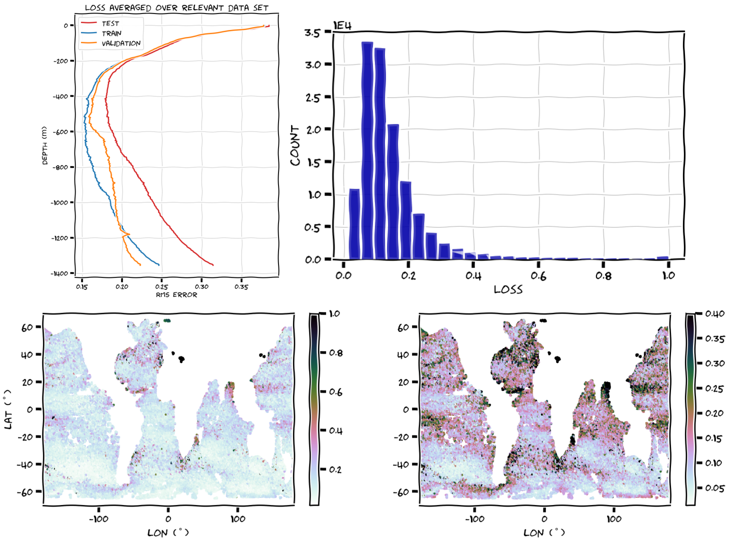


Figure: Some summary plots of the loss.

Neural Network

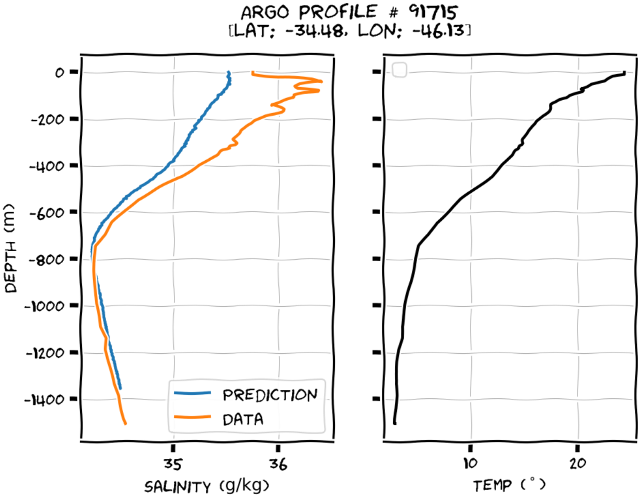


Figure: Example of a case with particularly high error.

Jupyter notebook

bonus Jupyter notebook (with thanks to Fei Er) to get some code practise

- different ways of reading the argo data
- different algorithms to try
- different questions to ask
- different features to add

  → those based on topology?
- ...

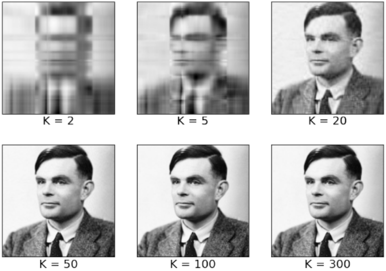


Figure: Image reconstruction: Neural network with data from PCA?