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  `https://github.com/julianmak/academic-notes`

  The repository principally contains the compiled products rather than the source for size reasons.
- Associated Python code (as Jupyter notebooks mostly) will be held on the same repository. The source data however might be big, so I am going to be naughty and possibly just refer you to where you might get the data if that is the case (e.g. JRA-55 data). I know I should make properly reproducible binders etc., but I didn't...
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OCES 3301 :

basic Data Analysis in ocean sciences

Bonus Session: Machine Learning

Outline

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

- a very loose introduction to Machine Learning (ML)

  $\rightarrow$ example with argo data

  $\rightarrow$ 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

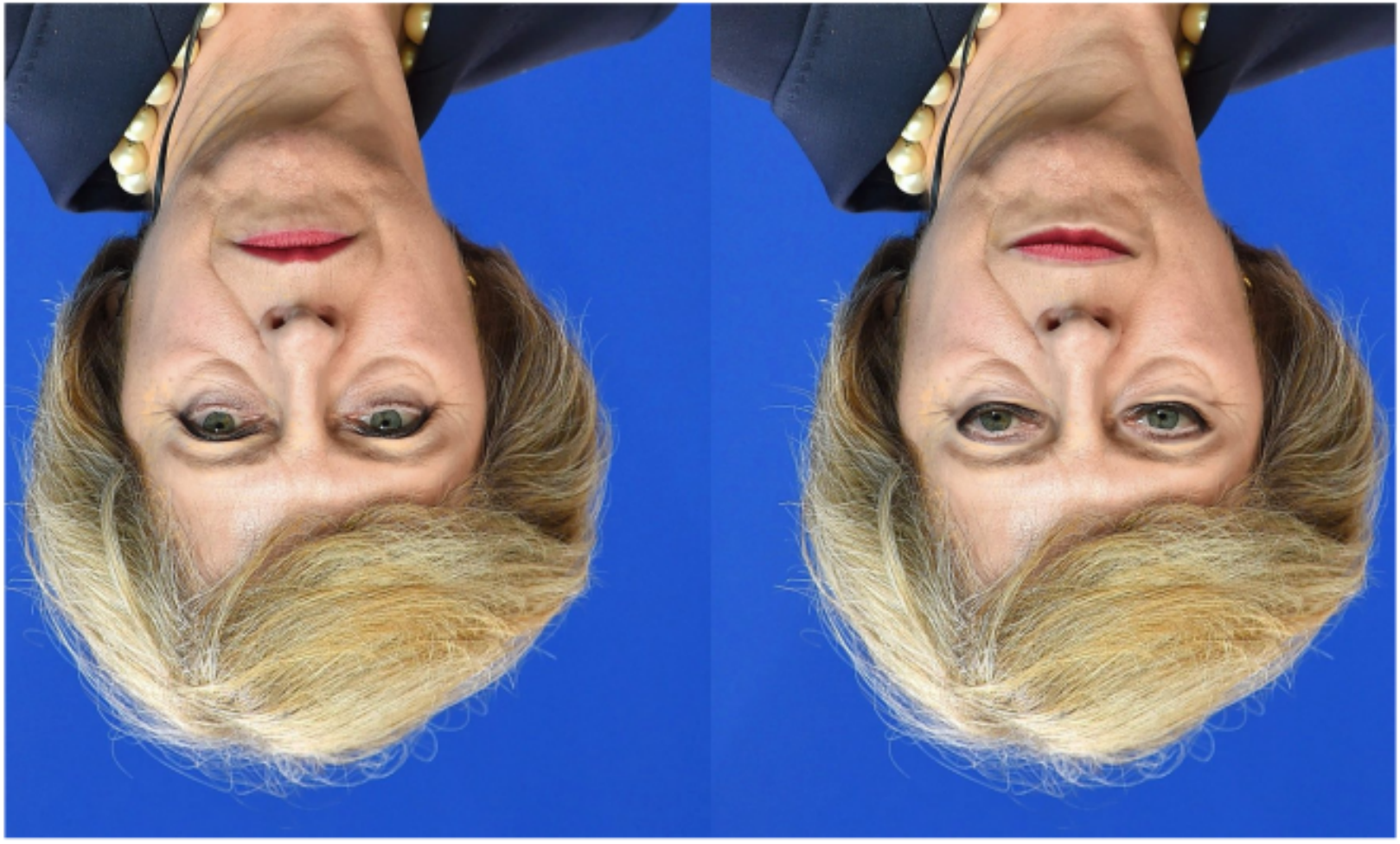


Figure: Cursed beast?

Cursed example: image recognition/generation

Figure: Cursed

Machine learning + regression/optimisation (see 03 + 04)

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

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

- ML in a nutshell follows the same principle

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

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.

Argo (see also lec 19 of OCES 2003)

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

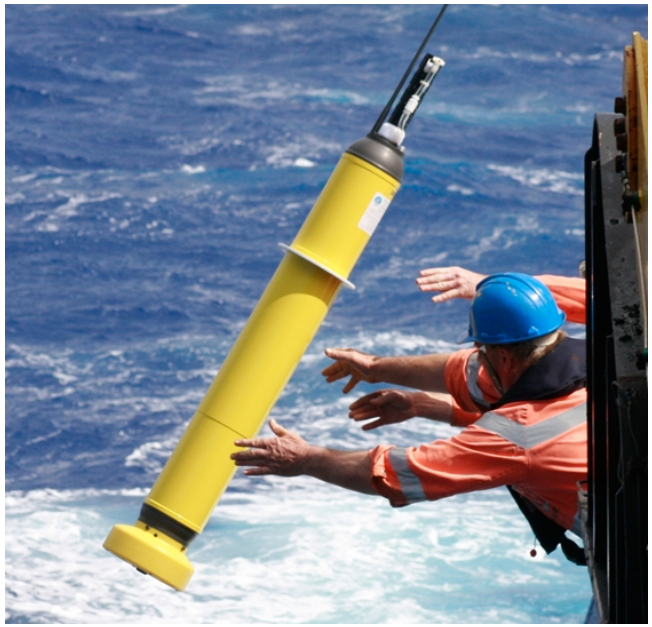


Figure: An Argo float being thrown off a ship. Image from NOAA.

Argo (see also lec 19 of OCES 2003)

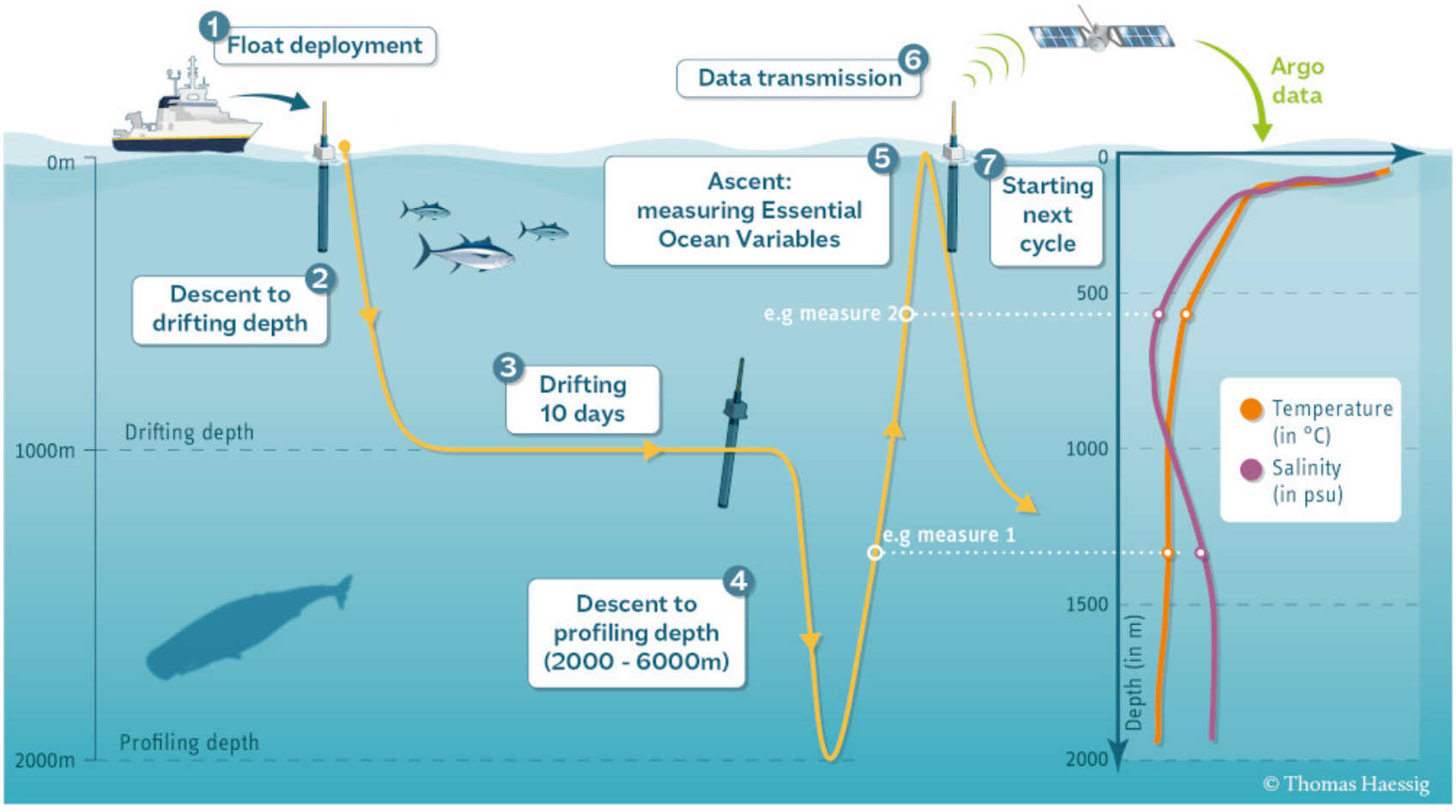


Figure: Argo float cycle schematic. From `argo.ucsd.edu`

Argo (see also lec 19 of OCES 2003)

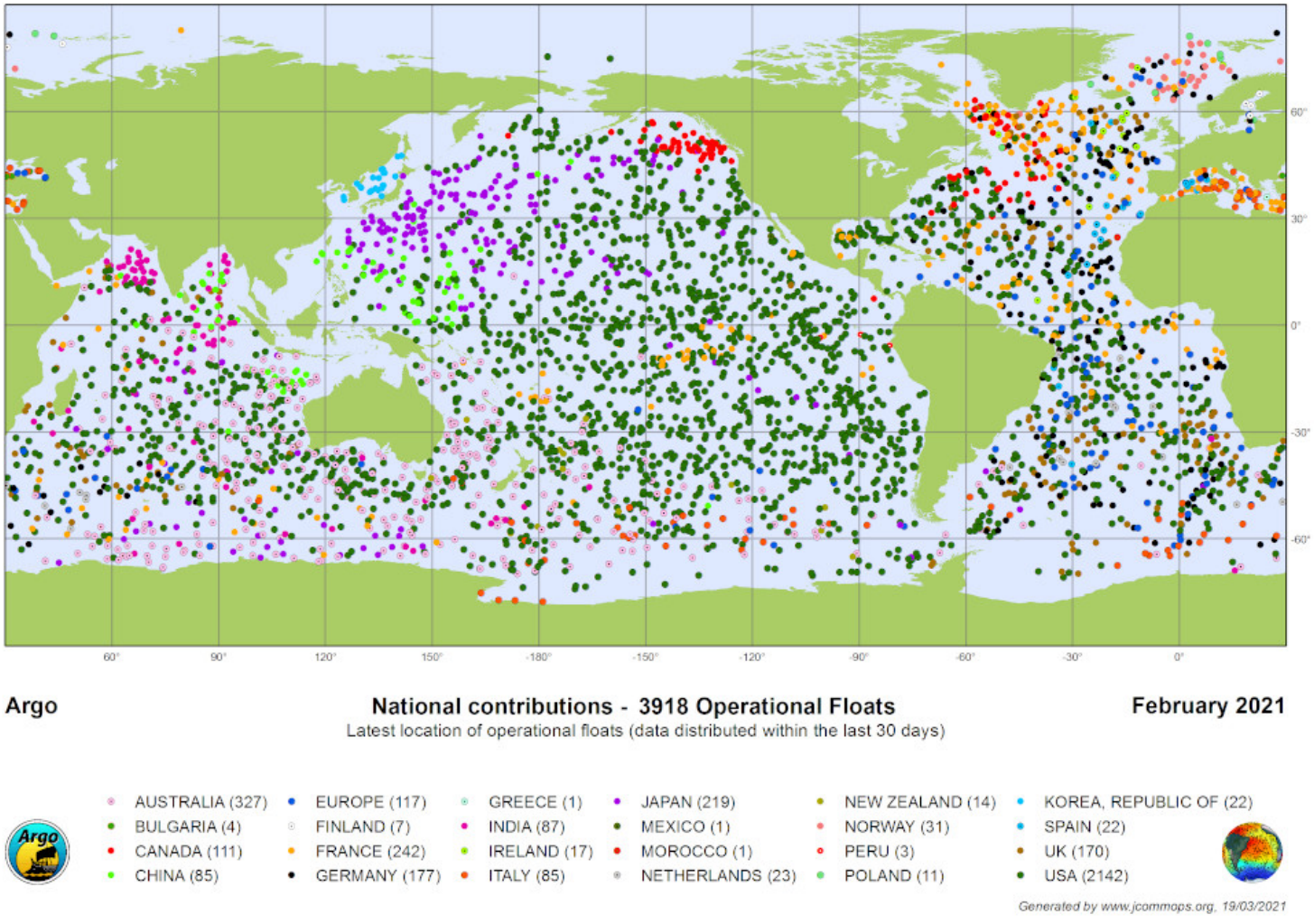


Figure: Argo locations as of Feb 2021. Note the dots are enhanced in size, so coverage is not as dense as it seems. From `argo.ucsd.edu`

Argo (see also lec 19 of OCES 2003)

▸ 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 here given in zarr format
  → need `zarr` package, can open data through xarray
  → ungridded data here
  → see also `argopy` package

Argo (see also lec 19 of OCES 2003)

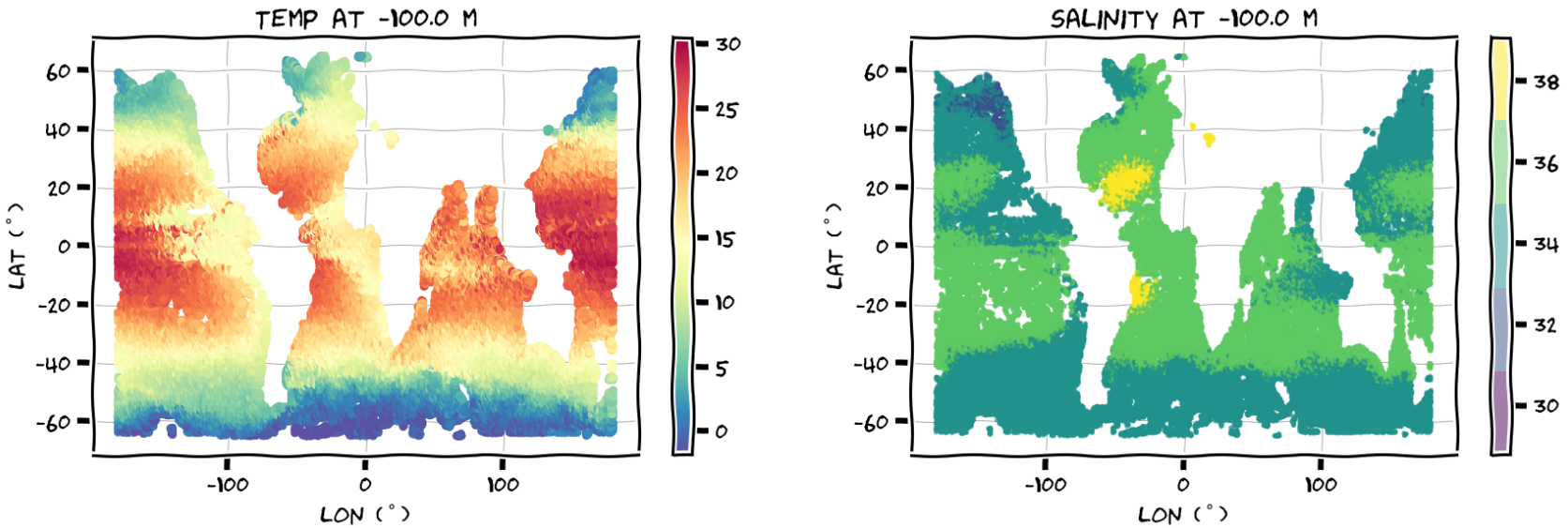


Figure: Argo (in-situ) temperature and (practical) salinity at some fixed depth as a scatter plot coloured by data entry.

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

Argo: clustering

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

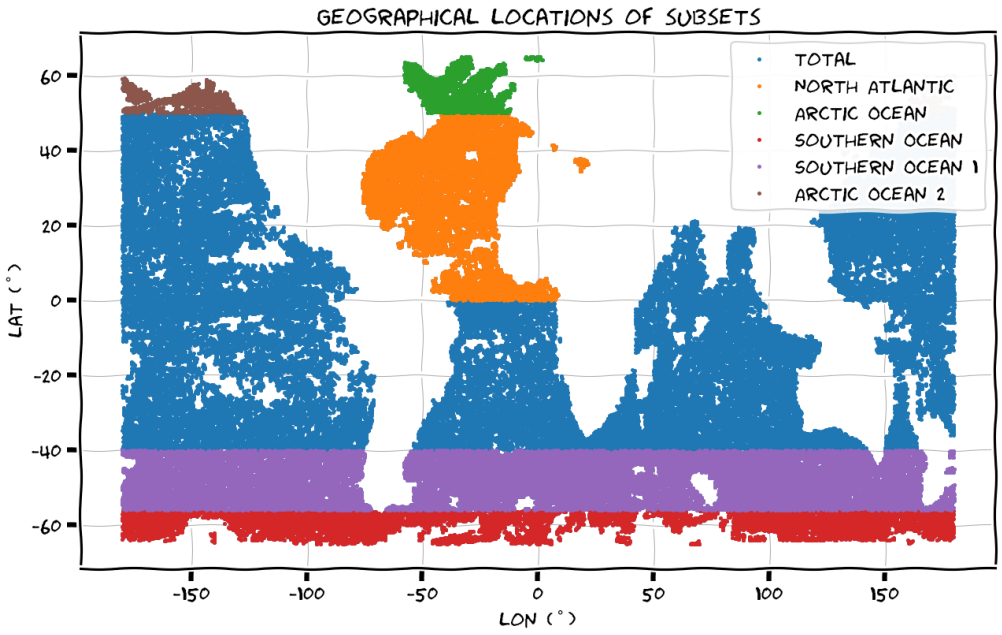


Figure: Artificial clustering.

Argo: clustering

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

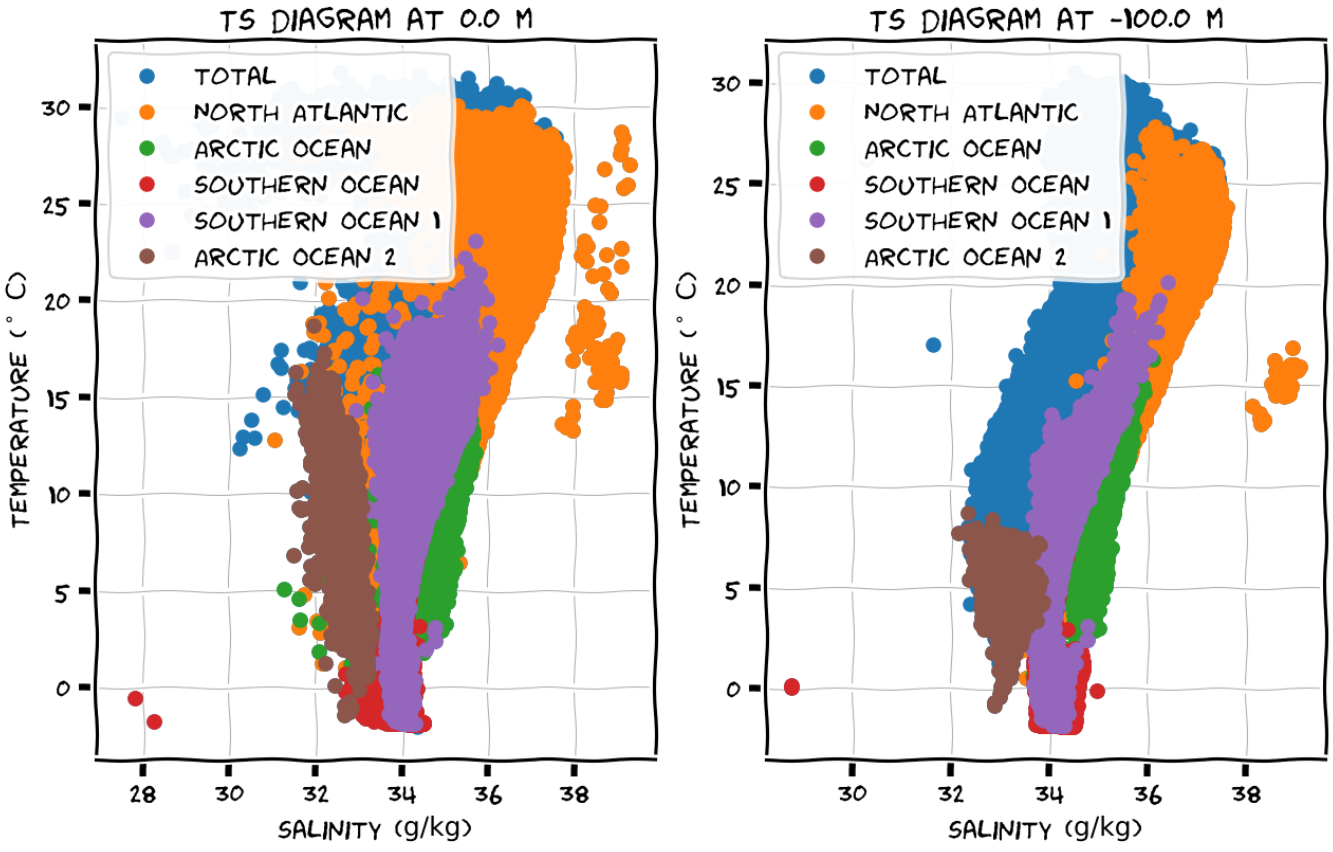


Figure: Artificial clustering as above, but in *TS*-diagram.

Argo: 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)

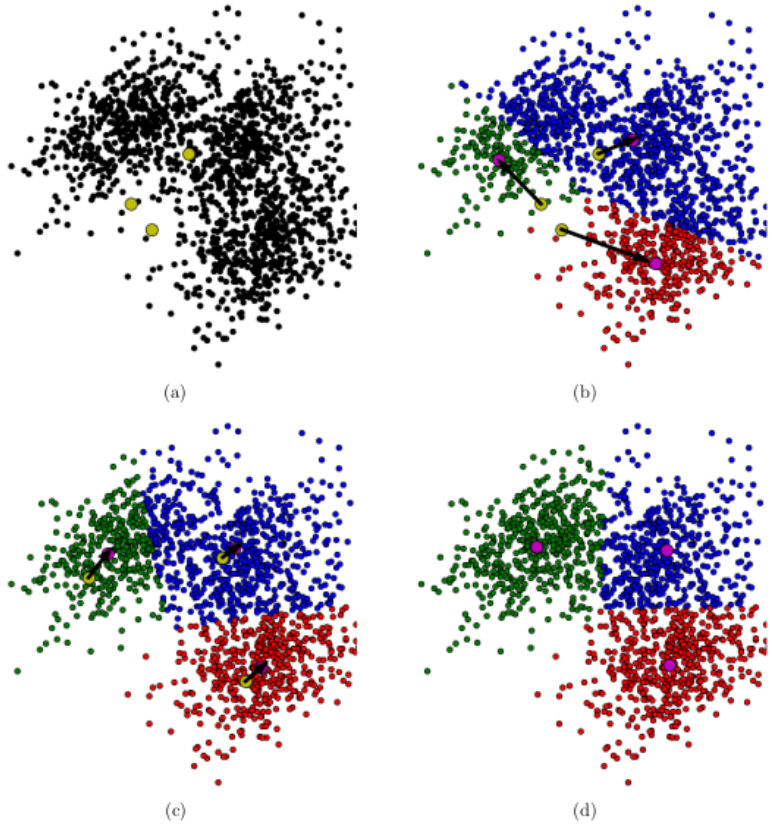


Figure: Demonstration of *k*-means algorithm. Diagram taken from Machine Learning course of Christoph Haase and Varun Kanade at University of Oxford.

Argo: clustering

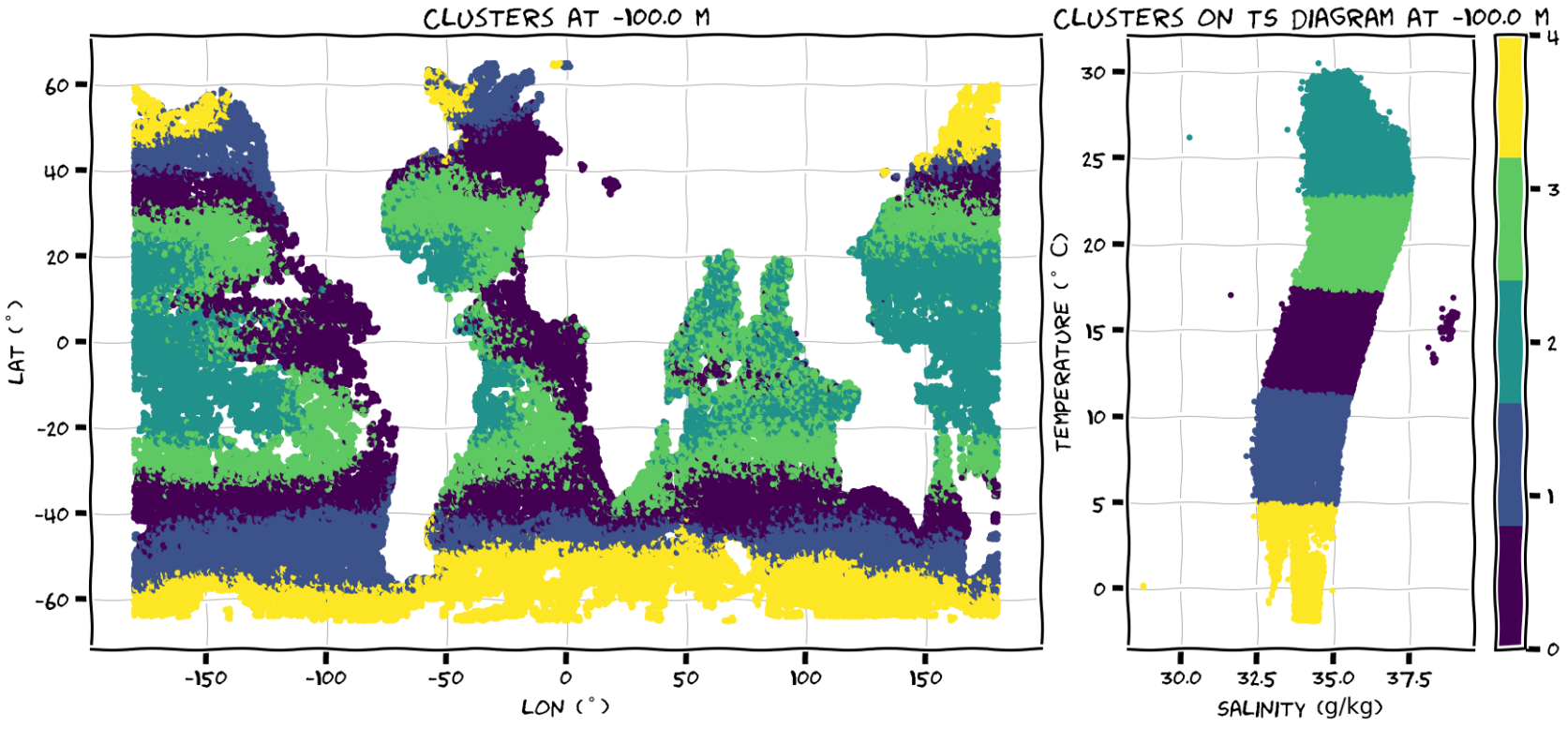


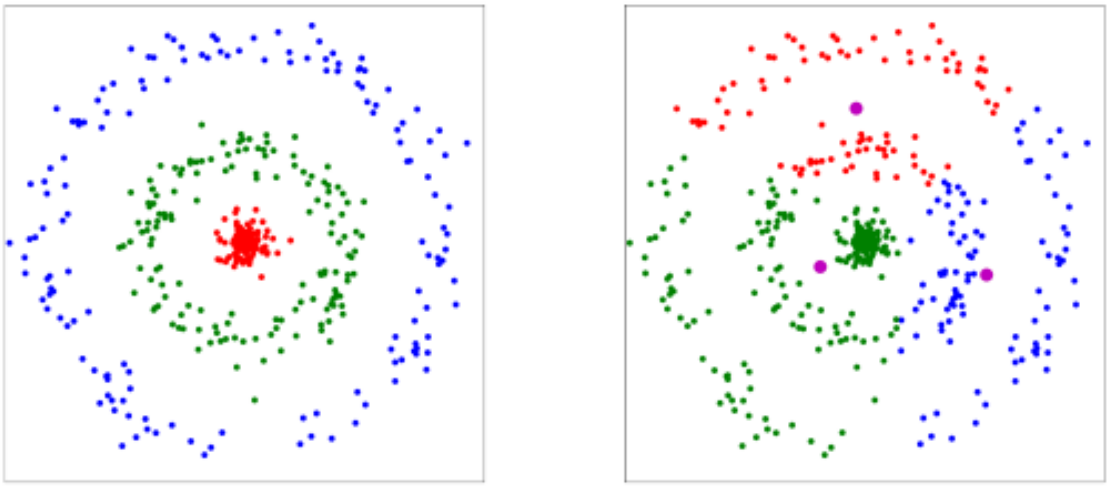
Figure: Clustering from *k*-means algorithm.

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

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

Argo: 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.

Argo: clustering

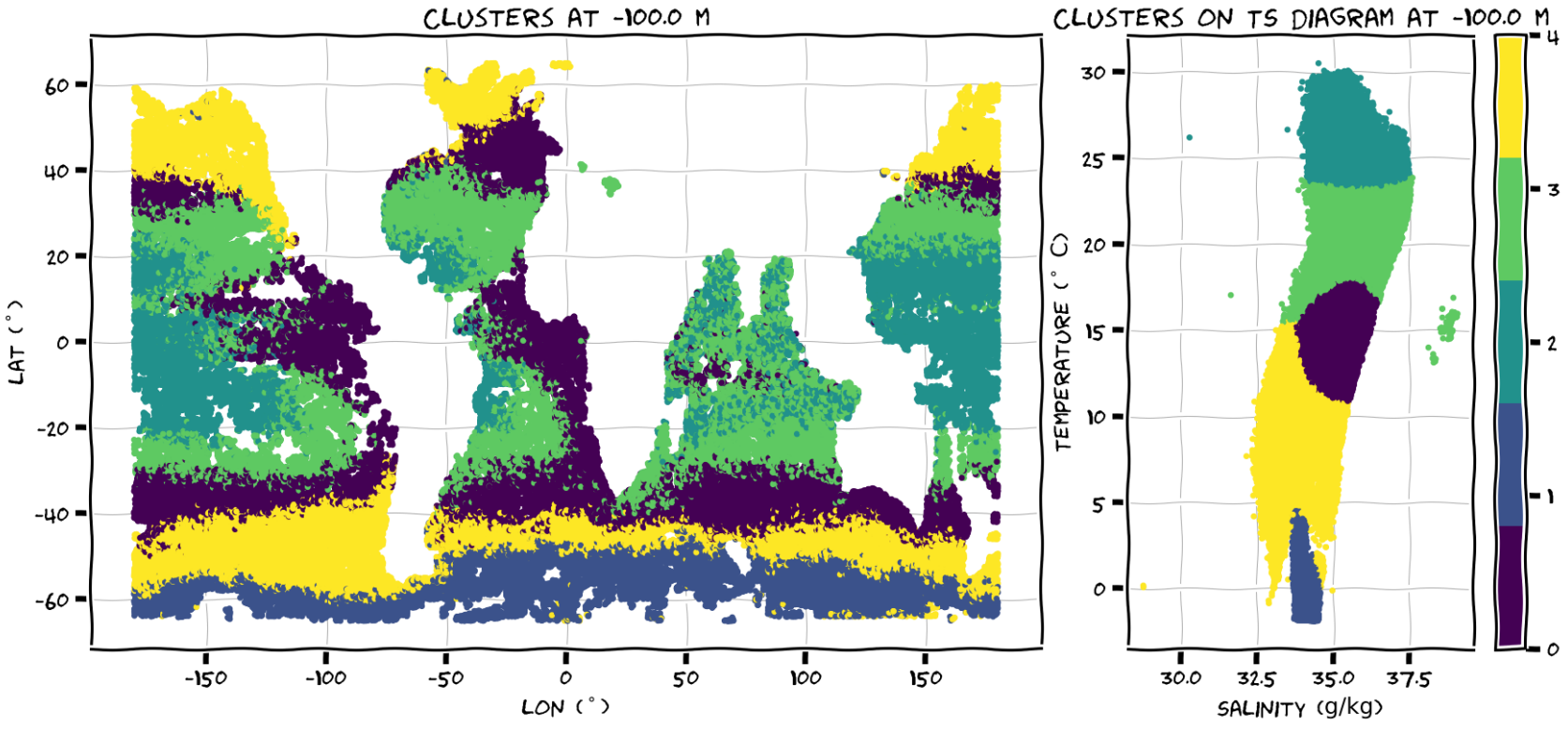


Figure: Clustering from Gaussian Mixture Model.

- 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)

Argo: neural network

- suppose we want to predict salinity from temperature
  → more for demonstration really...
  → split data first (`sklearn.train_test_split`)

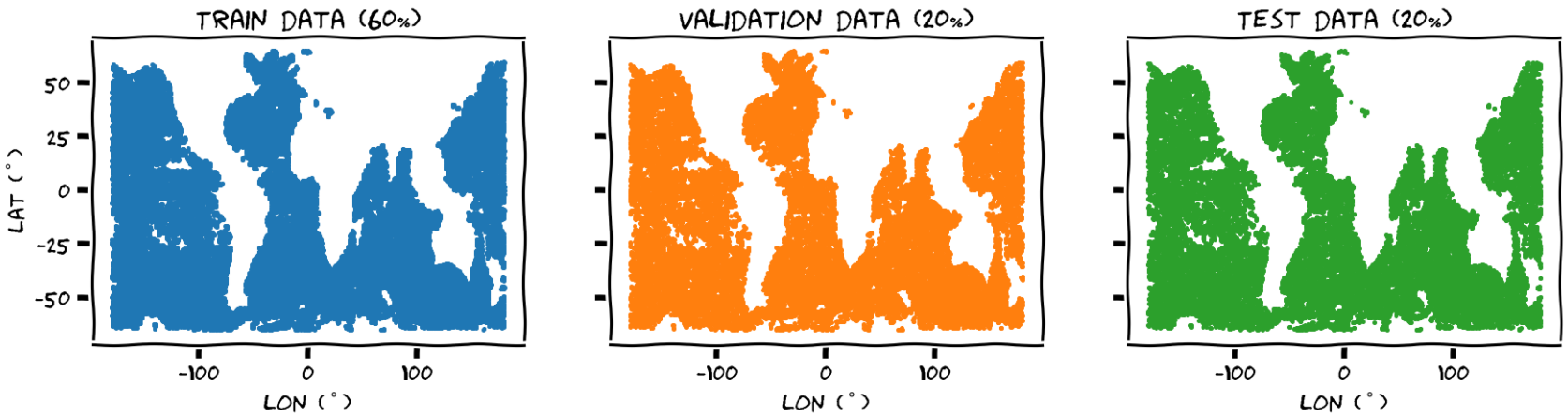


Figure: Splitting of argo data into training:validation:test as 60:20:20.

Argo: neural network

- linear regression?

  $\rightarrow$ standardise data

  $\rightarrow$ train with training data (could in principle use everything)

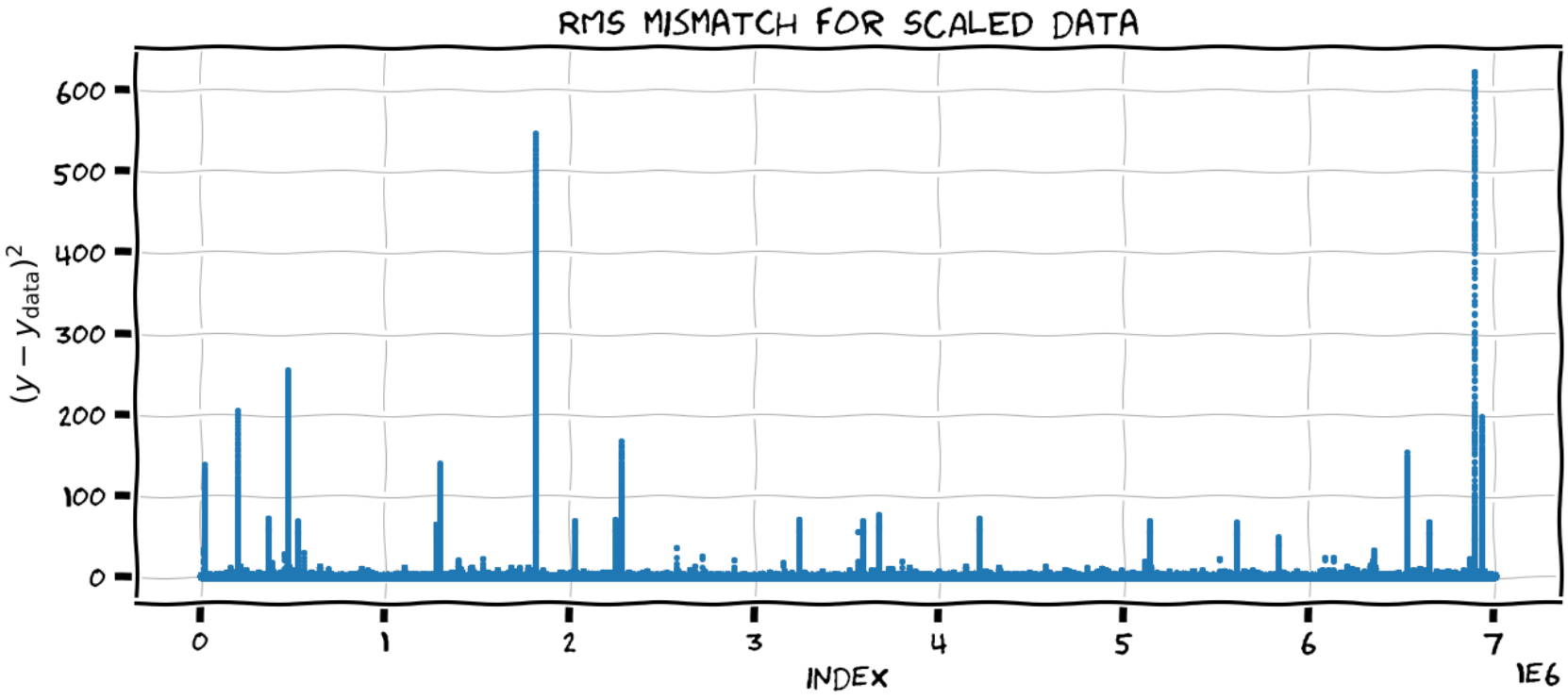
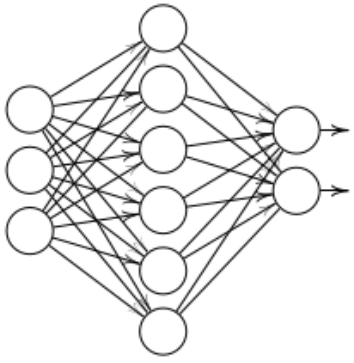
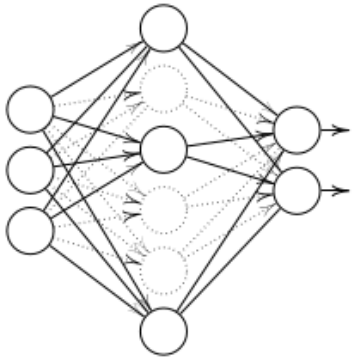


Figure: Root-mean-square loss against index for scaled data, so anything larger than 1 is pretty bad.

Argo: 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

Argo: 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

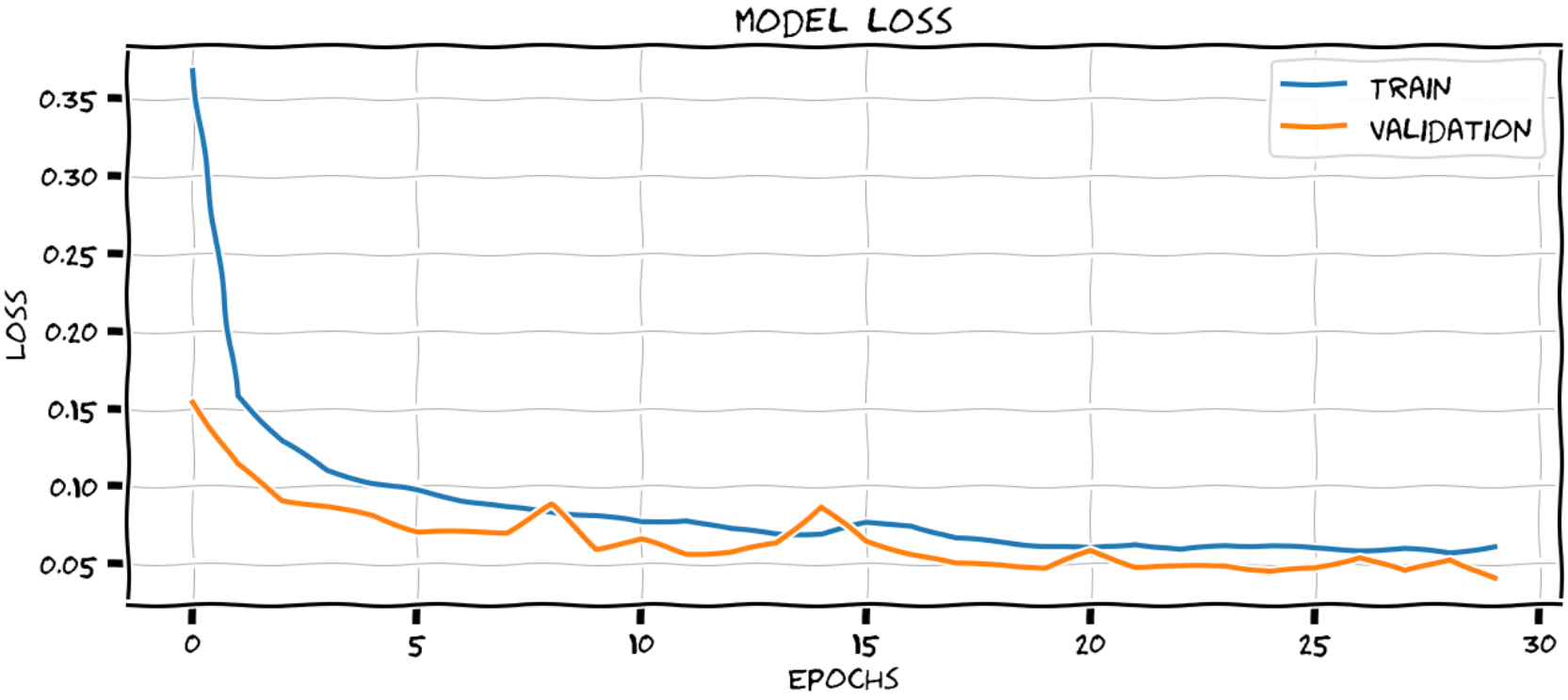


Figure: RMS loss against epoch. Note the RMS loss is not zero (and we don't expect it to be).

Argo: neural network

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

  $\rightarrow$ three random realisations below, with scaling inverted

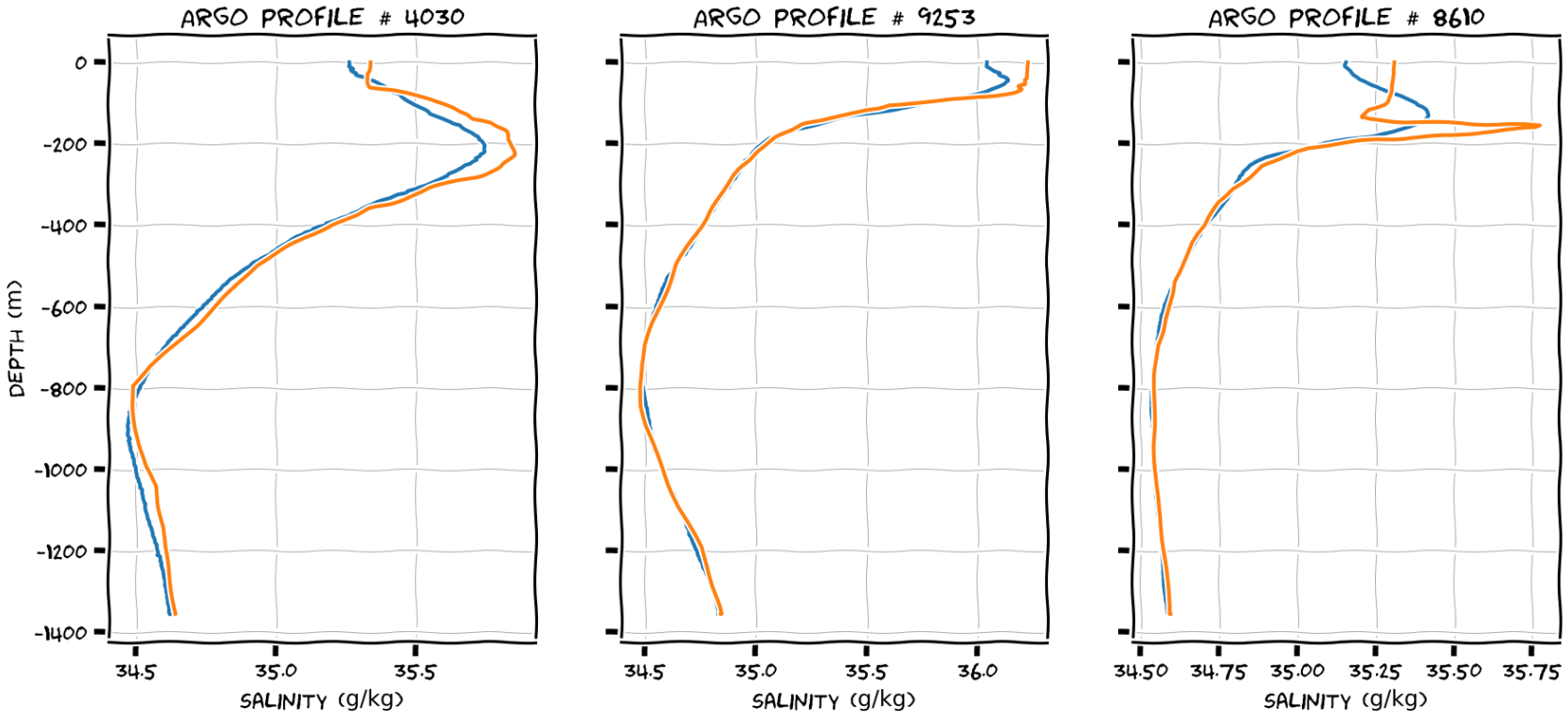


Figure: Three examples of using the trained neural network.

Argo: neural network

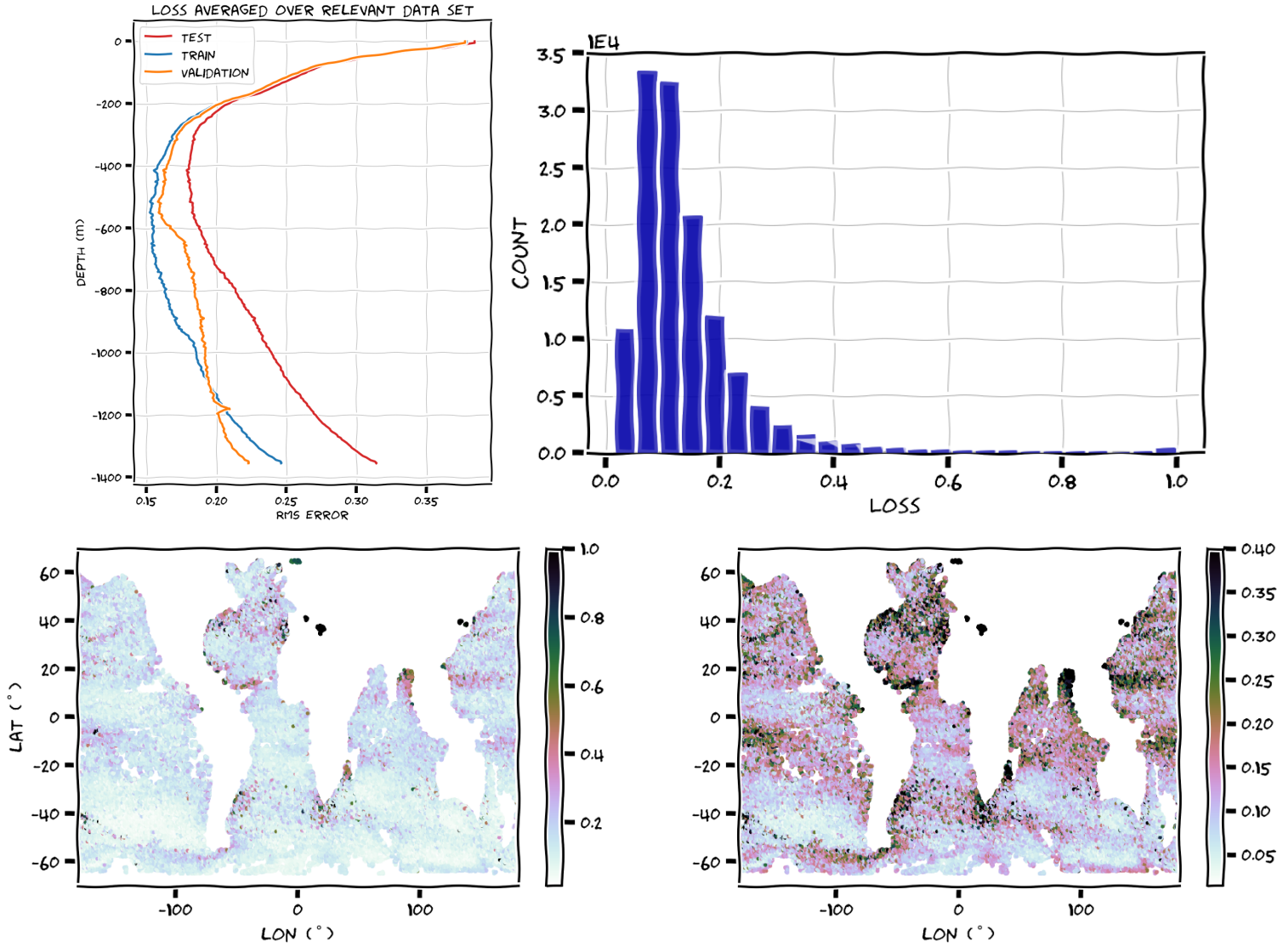


Figure: Some summary plots of the loss.

Argo: neural network

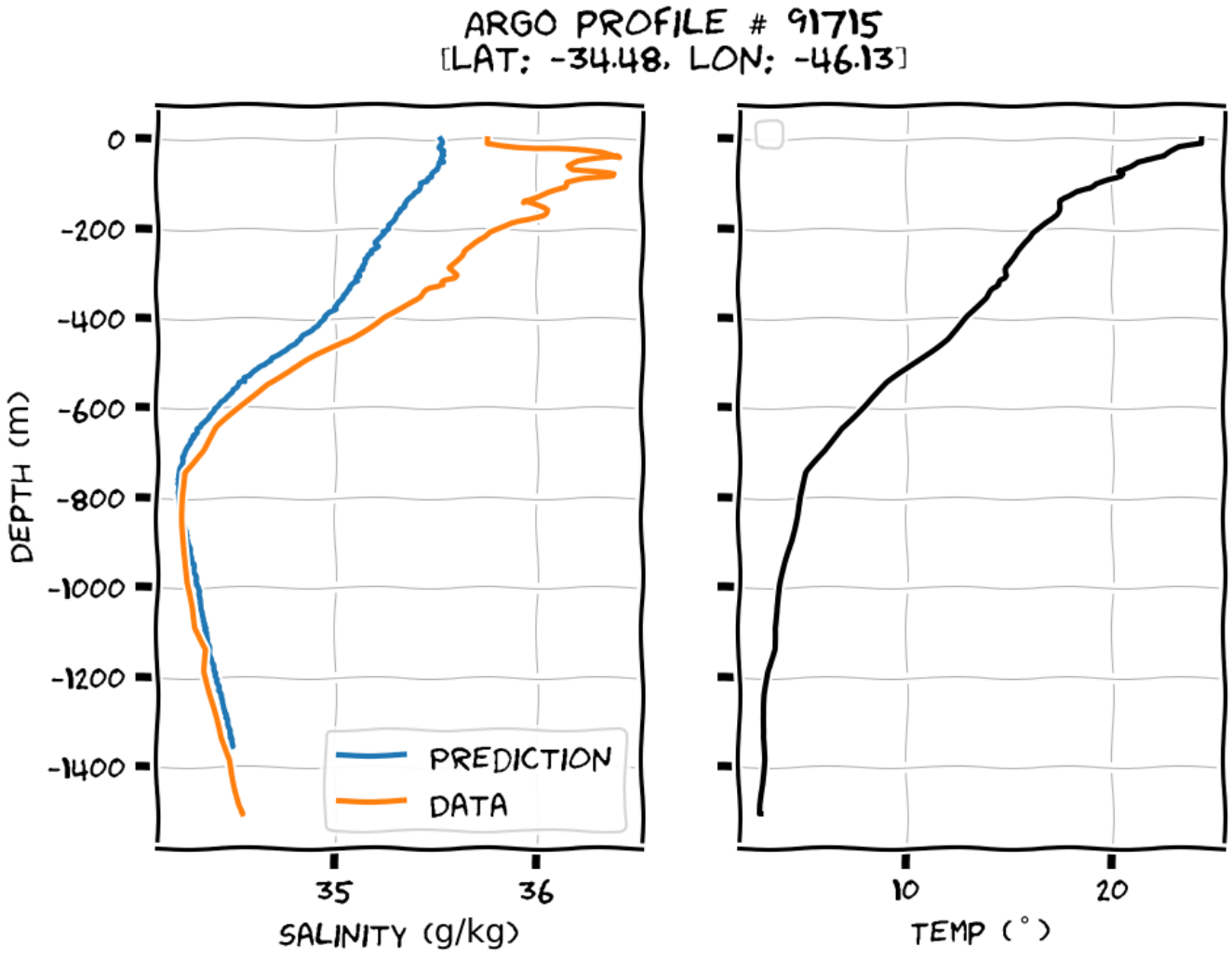


Figure: Example of a case with particularly high error.

Jupyter notebook

go to 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 datasets (e.g. Iris and/or Penguin)?
- . . .

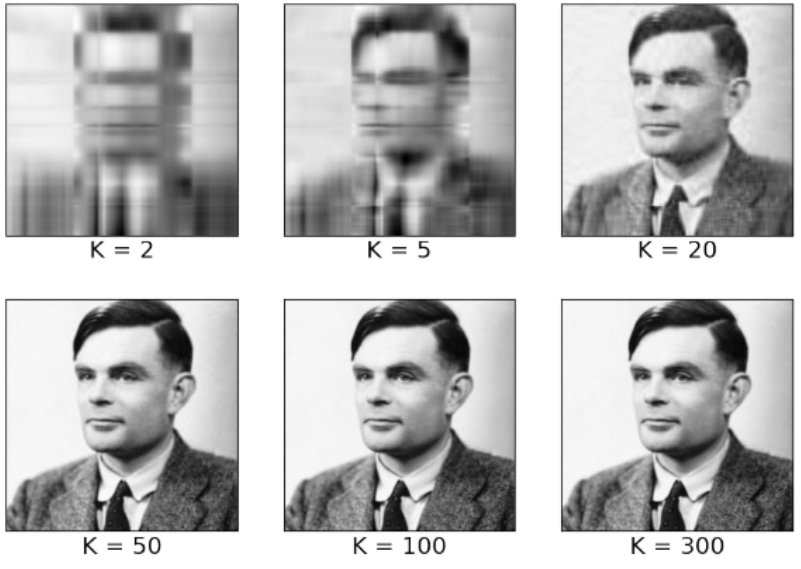


Figure: Image reconstruction (who is this person?) Neural network with data from PCA? (cf. exercise in 04, linear regression of data from PCA)