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  `https://github.com/julianmak/OCES5303_ML_ocean`

  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 5303 :
ML methods in Ocean Sciences

Session 2: more `sklearn`, cross-validation

Outline

- more `sklearn` things
  → linear models such as Linear Regression, Ridge, Lasso, Elastic-Net (cf. exercise in varing the loss function)
  → idea behind gradient descent
  → dimension reduction (e.g. PCA, lle, t-SNE)
  → clustering (e.g. K-means, others)

- cross validation and model hyper-parameter tuning
  → k-folds cross validation
  → ensemble methods

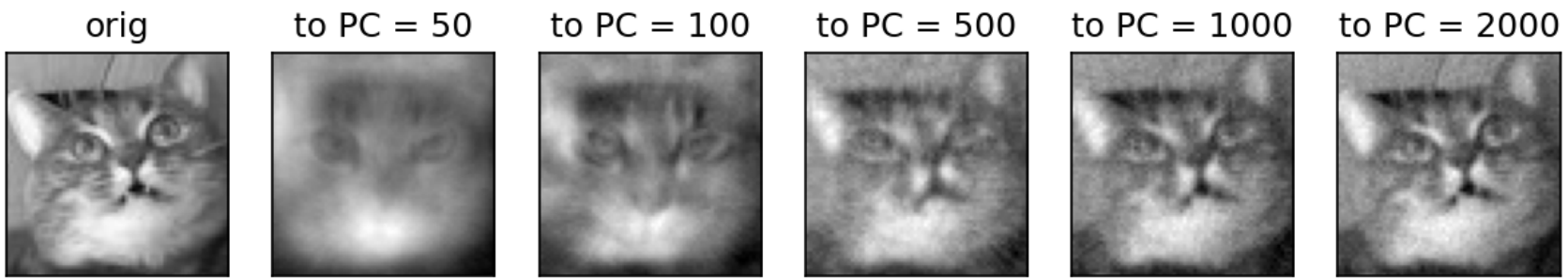

Figure: Result from an eigencat projection (it's really just PCAs).

Linear models

- given multiple features $X = (X^{(1)}, X^{(2)}, \ldots)$ and a **single** target Y, a linear model considers

$$\hat{Y} = a_0 + a_1 X^{(1)} + a_2 X^{(2)} + \ldots a_N X^{(N)}$$

  $\rightarrow$ the model parameters or control variables are $\{a_0, a_1, \ldots, a_N\}$

  $\rightarrow$ basically a linear algebra type problem (e.g. invert the matrices)

  $\rightarrow$ different methodologies take different loss functions J (see later)

- NOTE: this is not multi-variate regression where we have **multiple** targets Y, but see GLMs

Linear models: Linear Regression

- standard linear regression takes

$$J = \|\hat{Y} - Y\|_{L^2}^2 = \sum_{i=0}^{M} |\hat{Y}_i - Y_i|^2,$$

where Y_i is the training data and $\hat{Y}_i$ are the predictions from the model

$\rightarrow$ note lower index, M samples, but N lots of features described by $X^{(j)}$

$\rightarrow$ this basically provides the 1d LOBF embedded in $(N+1)$d space

$\rightarrow$ can have issues when features (the $X^{(j)}$) are not independent of each other

$\rightarrow$ can be sensitive to data noise

Linear models: Ridge

- consider controlling the size of the model coefficients a by

$$J = \|\hat{Y} - Y\|_{L^2}^2 + \alpha \|a\|_{L^2}^2$$

$\rightarrow$ this is peanlisation on a with strength α

- extra hyper-parameter α here

$\rightarrow$ large α means small coefficients and control colinearity, but at then expense of skill

- NOTE: different α's needed if data is not standardised

Linear models: Lasso

- could even limit number of features by asking for as many zero a_j as possible, via

$$J = \frac{1}{2M} \|\hat{Y} - Y\|_{L^2}^2 + \alpha \|a\|_{L^1}$$

$\rightarrow$ large α we want to keep as many non-zero coefficients as possible, but at then expense of skill

$\rightarrow$ relations to **compressed sensing**

Linear models: Elastic-nets

- could do a bit of both via

$$J = \frac{1}{2M}\|\hat{Y} - Y\|_{L^2}^2 + \alpha\rho\|a\|_{L^1} + \frac{\alpha(1-\rho)}{2}\|a\|_{L^2}^2$$

$\rightarrow \rho$ is a ratio hyper-parameter controlling sparsity and model parameter values

Sample loss function + gradient descent

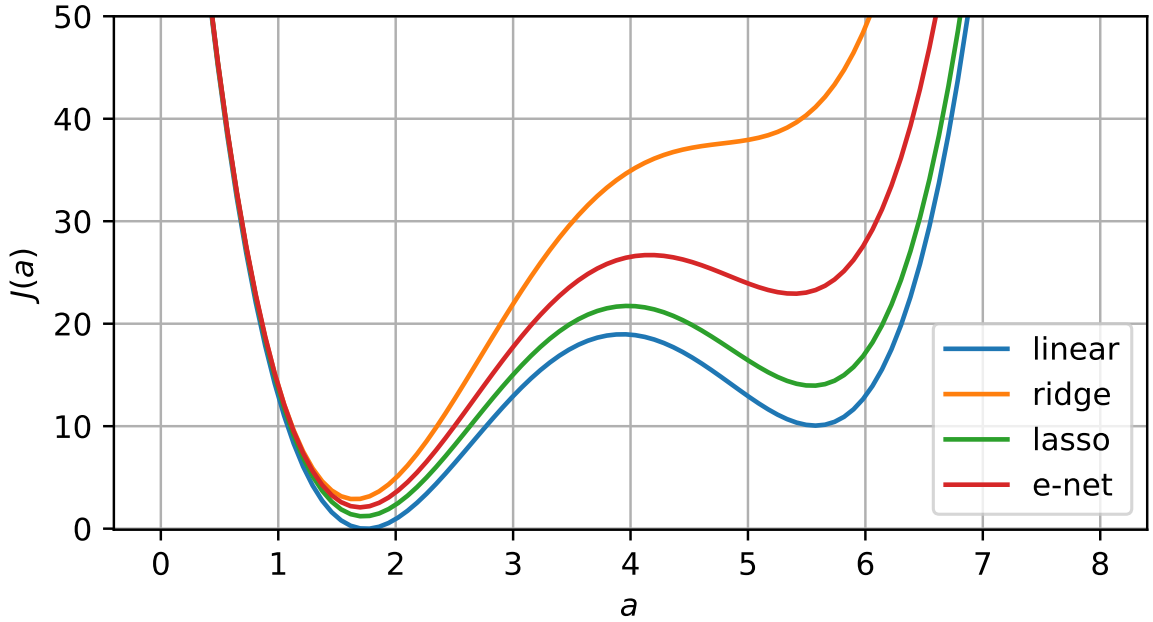

Figure: Made up 1d example of $J = J(a)$ with different choices of regularisation, $J = (1/2M)\|\hat{Y} - Y\|_{L^2}^2 + \alpha\rho\|a\|_{L^1} + (1/2)\alpha(1-\rho)\|a\|_{L^2}^2$.

- optimise by finding minimum, extremum occurs where the derivatives are zero $\Rightarrow$ root finding problem

  $\rightarrow$ **gradient** information is used to find direction of **descent**

Example: regressing to polynomial data

- going to do a demonstration case of taking

$$Y = X^2 + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \sigma)$$

where σ controls the level of 'noise', but going to fit this to

$$\hat{Y} = a_0 + a_1 X^1 + a_2 X^2 + \ldots a_{10} X^{10}$$

i.e. my features $X^{(j)}$ in this case happens to polynomials X^j (X raised to power j)

$\rightarrow$ might expect to get $a_2 = 1$ and small values elsewhere

$\rightarrow$ a slightly more subtle meaning to "linear" is needed...

Example: regressing to polynomial data

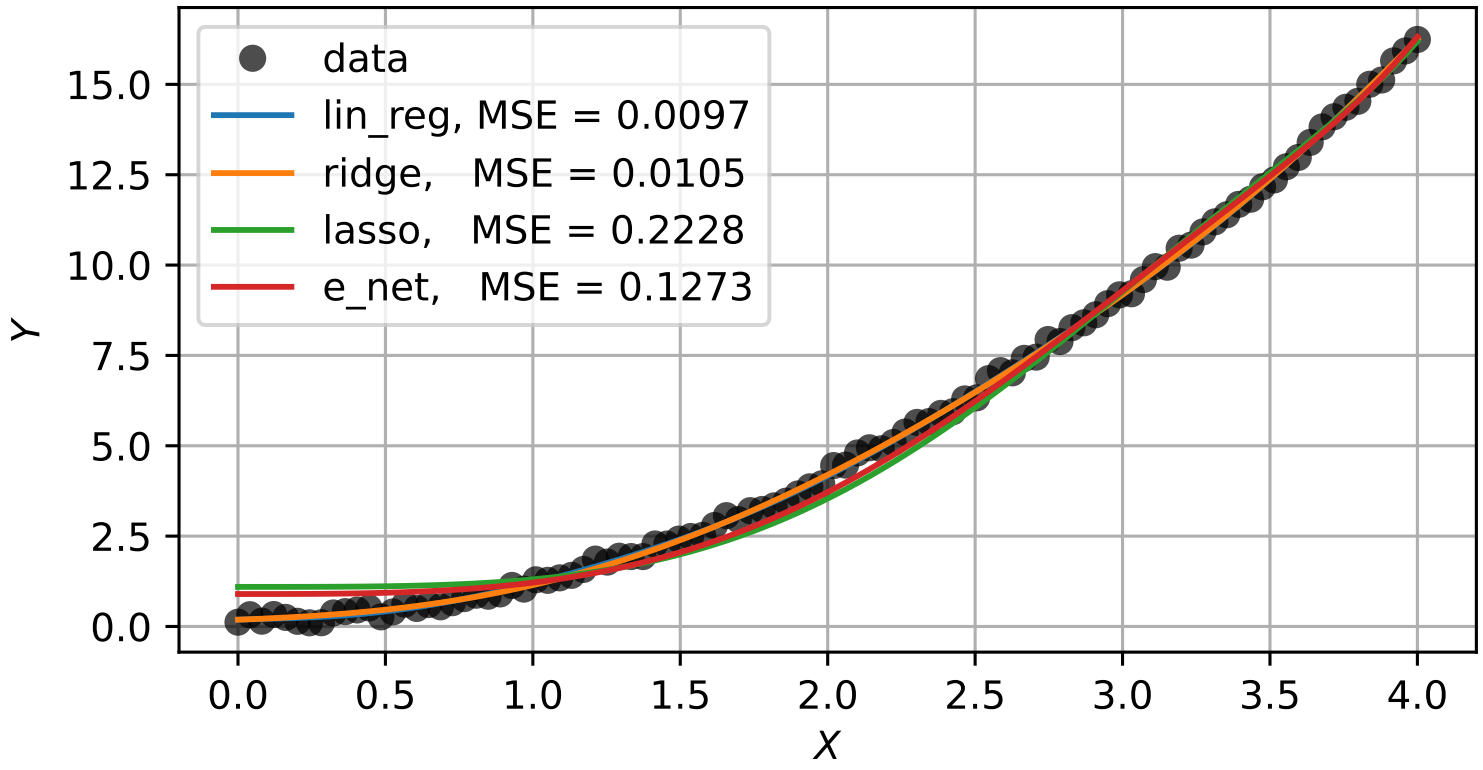

Figure: Polynomial regression for some contrived data, with MSE scores printed on.

Example: regressing to polynomial data

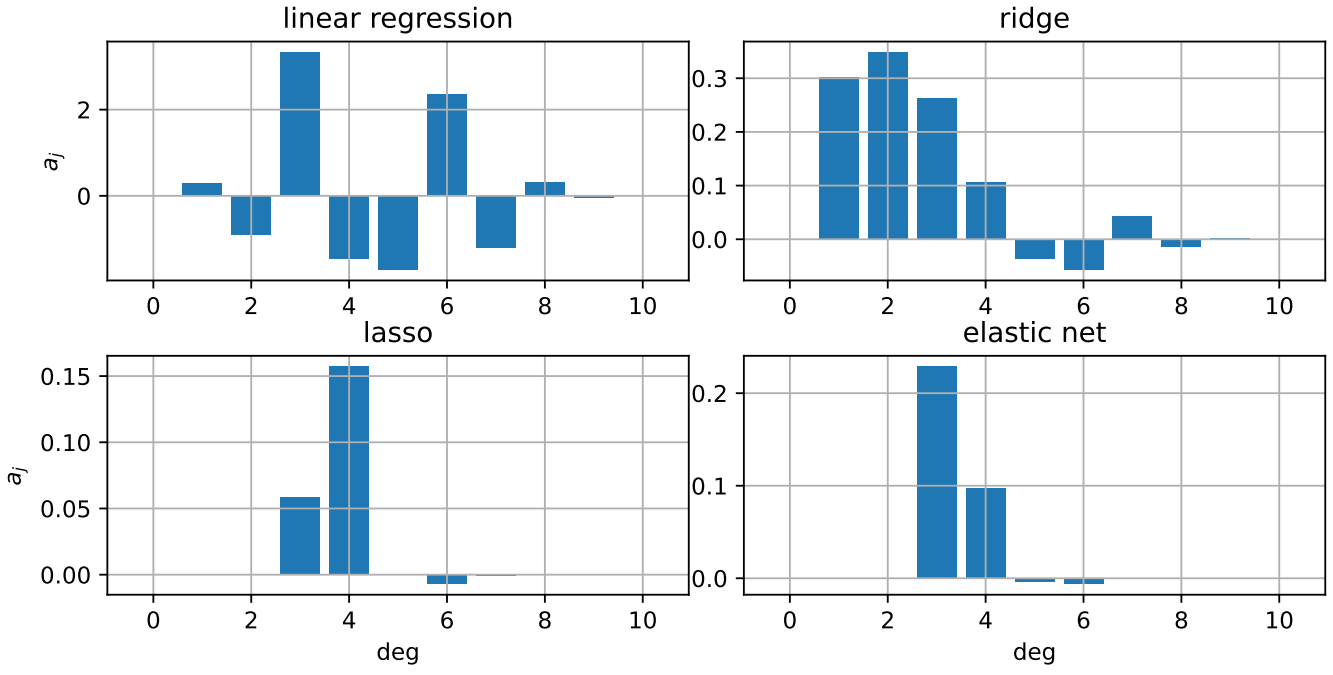

Figure: Polynomial regression for some contrived data, with MSE scores printed on.

- notice a_2 is not always largest!
- notice L^1 based penalisation (lasso and elastic net) gives more small coefficients

  $\rightarrow$ fewer features (more likely not over-fitted?)

Example: image classification + perceptrons (see Lec 04)

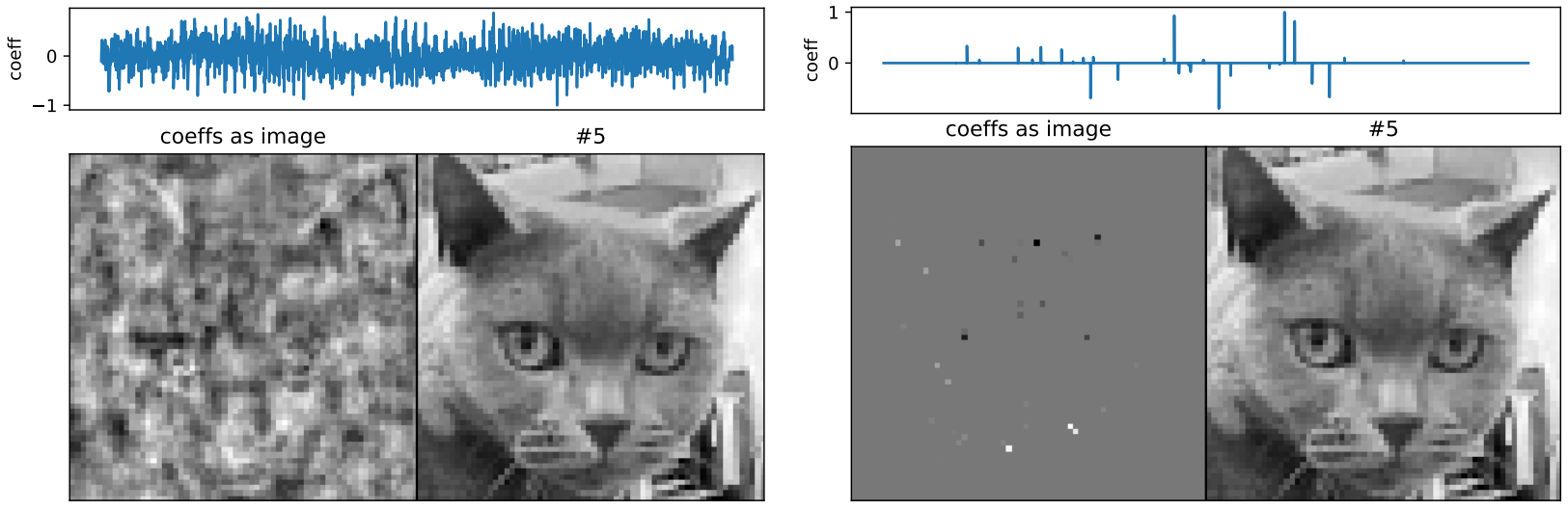

Figure: Visualisaing a perceptron from a pseudo-inversion of a matrix. (Left) Standard linear regression (L^2 inversion). (Right) Lasso (L^2 with a L^1 penalisation). See Lec 04.

- neural networks in its simplest form is just matrix inversion if the activation function is trivial

  $\rightarrow$ can obtain the model via a (pseudo-)inversion

  $\rightarrow$ basically an optimisation problem, can design loss functions accordingly

Dimension reduction: PCAs

Q. if not all features are as important, can find the important ones *a priori*?

$\rightarrow$ would help presumably against over-fitting

Dimension reduction: PCAs

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$\rightarrow$ would help presumably against over-fitting

- Principal Component Analysis (PCA) is one way

  $\rightarrow$ shows up also as Empirical Orthogonal Functions (EOFs) particularly when pattern are involved
- considers linear combinations of features that explain the most variance in the data

  $\rightarrow$ effectively does a SVD, returns
  1. singular values σ (related to variance explained)
  2. the left and right singular vectors that gives the new co-ordinate system and relevant expansions

Dimension reduction: PCAs

- easier to explain visually with the penguins
  $\rightarrow$ data has been standardised here

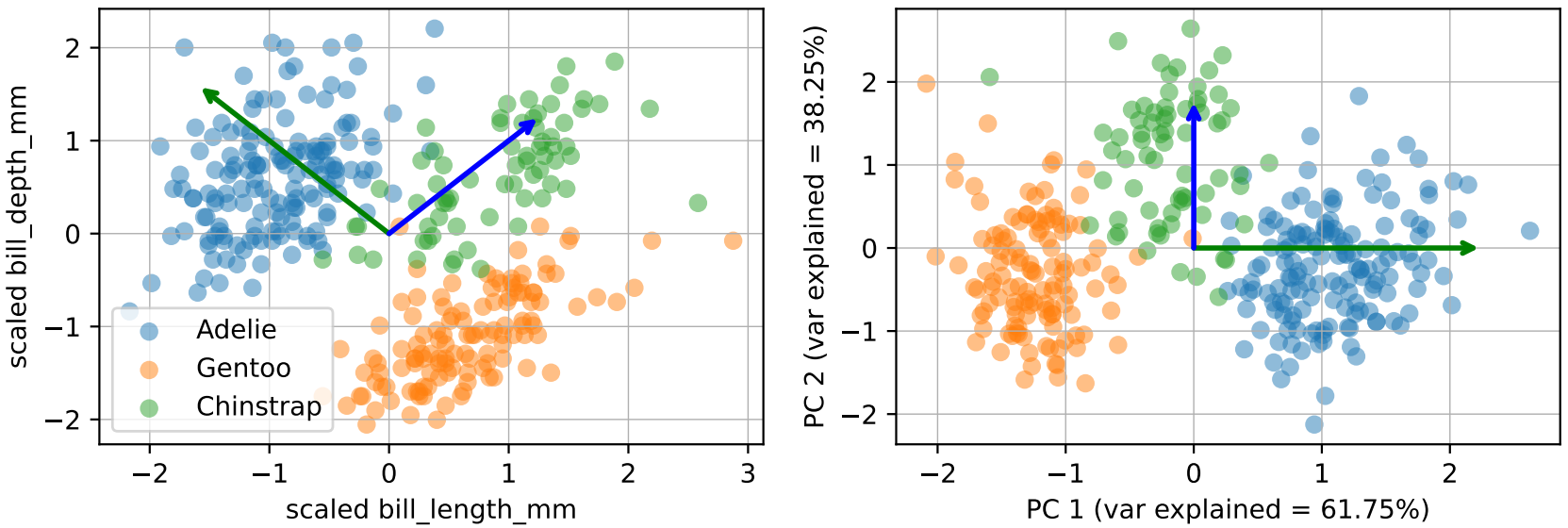


Figure: (Left) Original (but standarised) data with two choices of variables. (Right) The same but in the principal component representation.

- for this case it really is just a co-ordinate transformation

Dimension reduction: PCAs

- below shows dimension reduction (from 4 to 2)

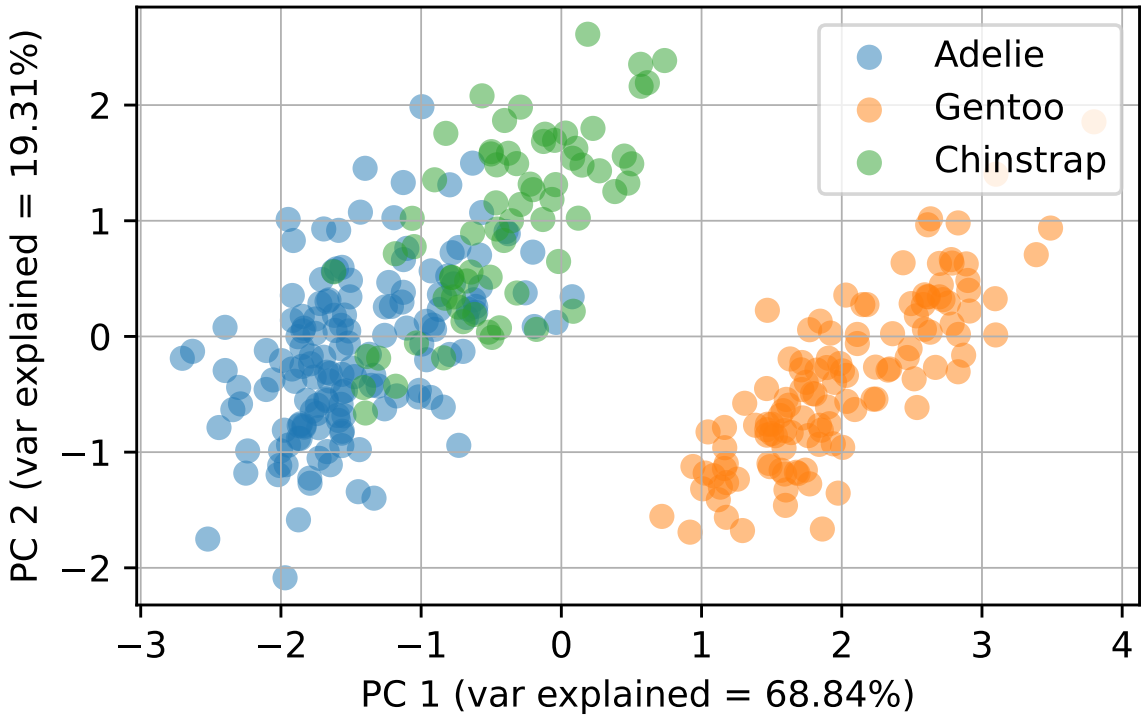


Figure: Representation in PC1 and PC2 co-ordinate system.

- note the variance explained does not sum to 100% here
  → this is now a **projection** which loses information

Dimension reduction: manifold methods

(This part makes more sense in about 15 mins)

- other manifold based methods

  → Locally Linear Embedding (preserves local distances, think local PCAs to give global co-ord)

  → *t*-distributed Stochastic Neighbor Embedding (*t*-SNE; based on pdfs, good at picking out local structures)

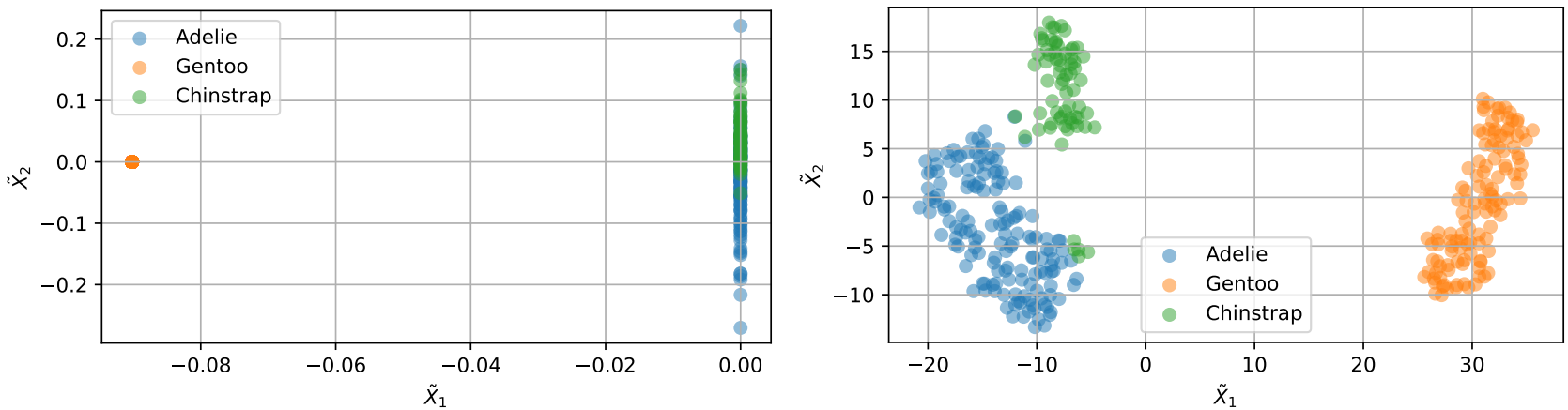


Figure: Demonstration of Locally Linear Embedding and *t*-SNE on the penguins data.

Demonstration: eigencat

- example demonstrating PCA on images of cats

  $\rightarrow$ feature extraction, cf. facial recognition
- massage data into `(n_cat,pixels)` then throw into PCA

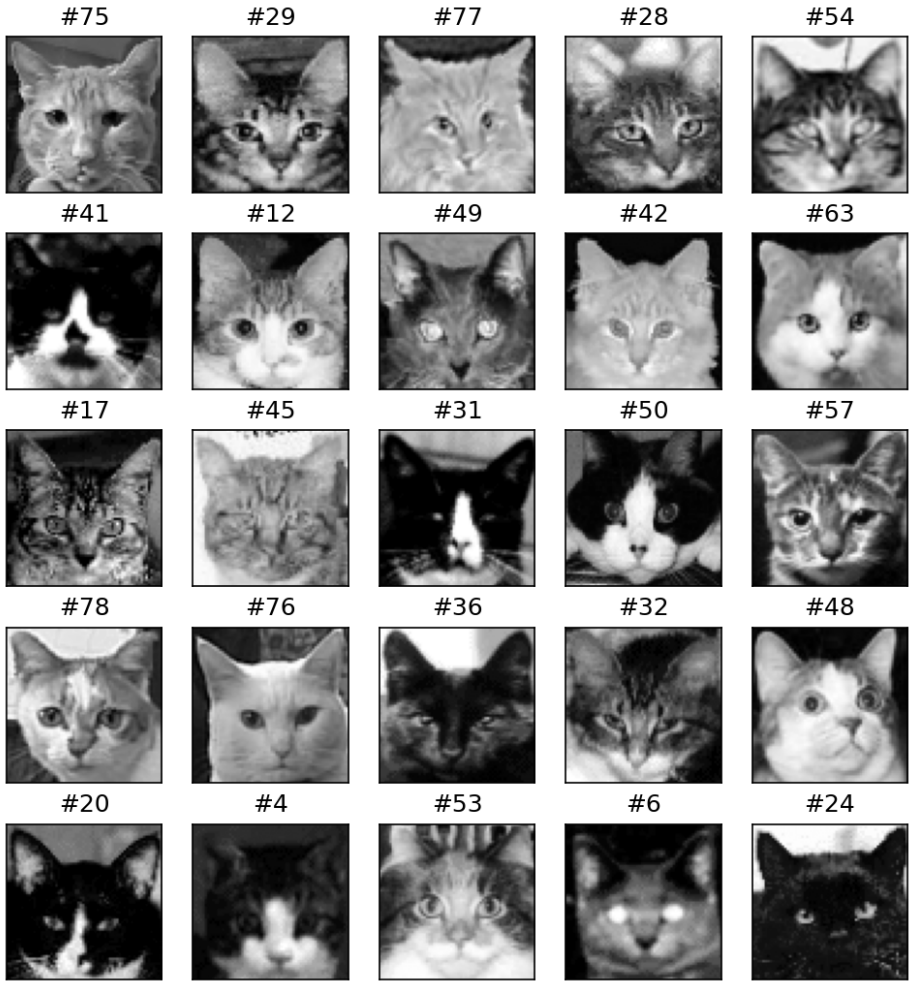


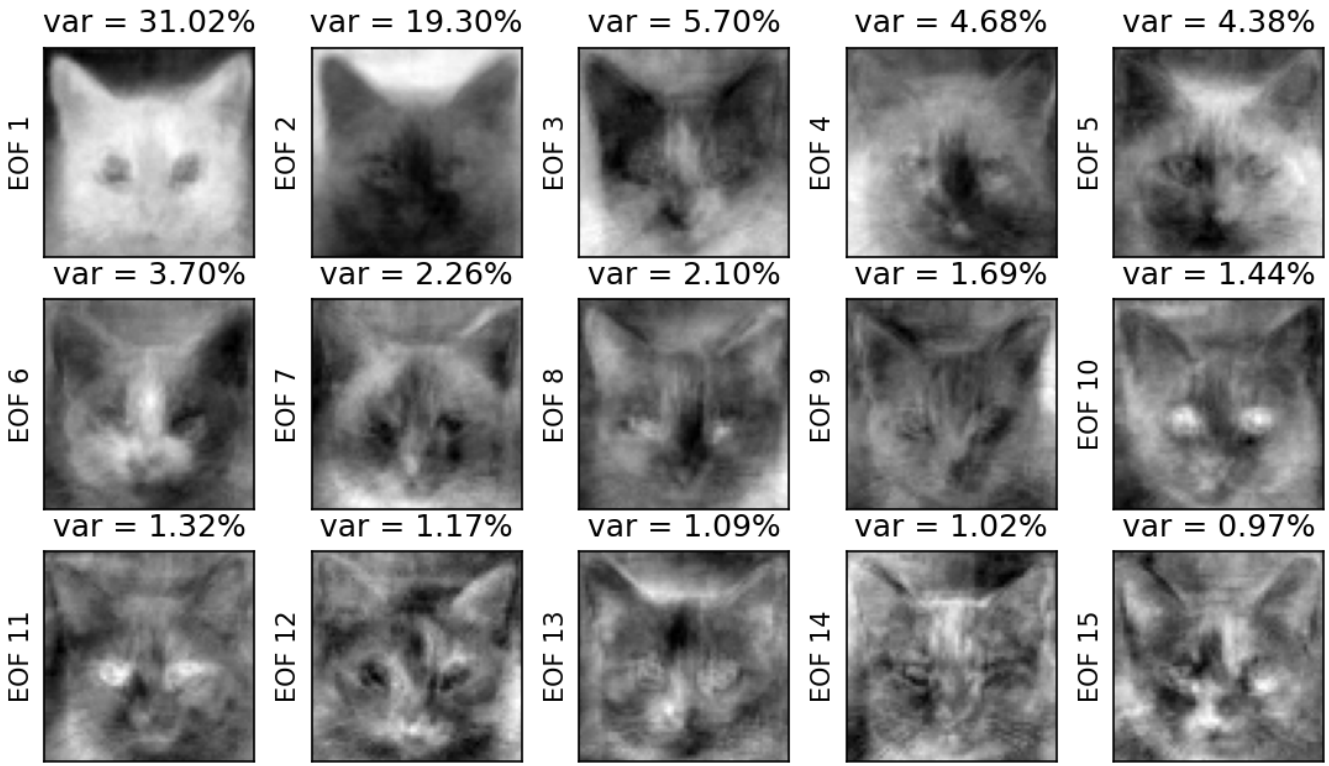
Figure: Data in `cats.csv`.

Demonstration: eigencat

- want

$$\text{Image}(\text{pixels}) = \sum_i \text{PC}_i \times \text{EOF}_i(\text{pixels}),$$

$\rightarrow$ call the patterns the EOFs, PCs are the loadings
$\rightarrow$ reshape EOFs to get "averaged" cat faces



Demonstration: eigencat

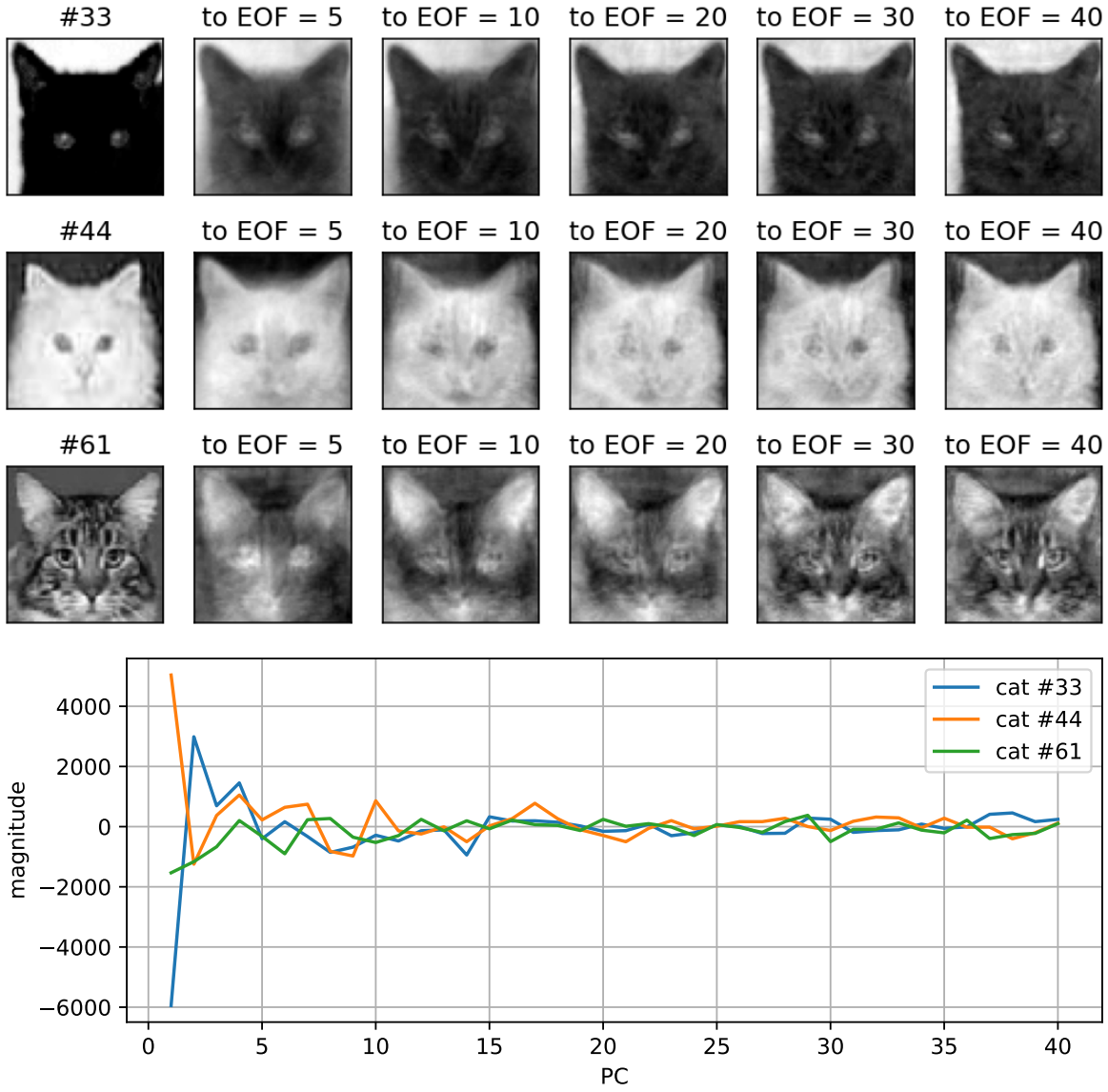


Figure: Expansion and loadings of three of the samples.

Demonstration: eigencat

- different cats will have a different PC pattern, use that as

  $\rightarrow$ signature for classification?

  $\rightarrow$ features for model training? (much lower dimension)

- warning: can start doing ridiculous things like below if my data space is large enough!

  $\rightarrow$ next few pages show the same thing if I use an expanded dataset (2000 images)

Demonstration: eigencat

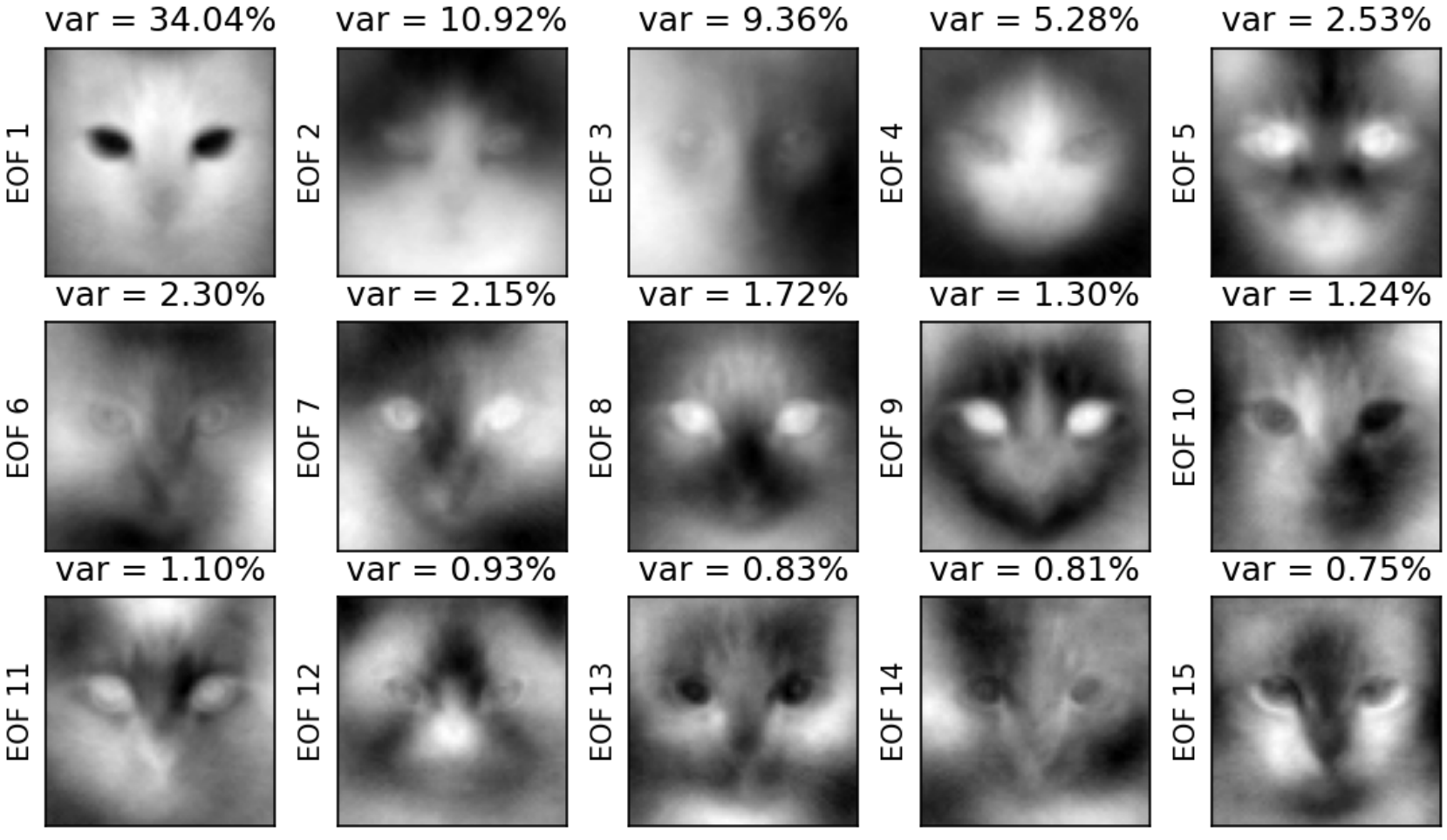


Figure: Eigencats from `cats_bw_enlarged.csv`.

Demonstration: eigencat

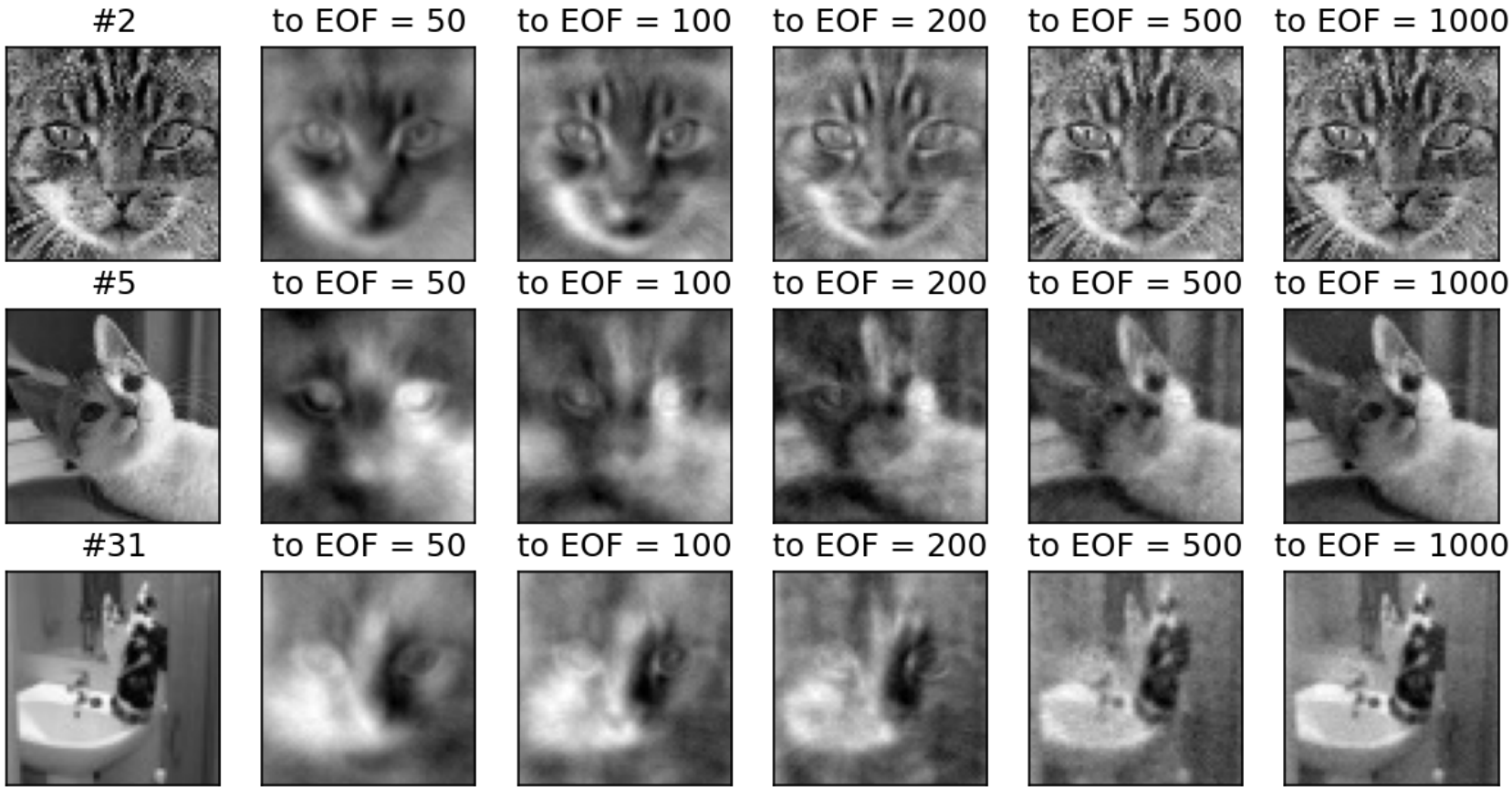


Figure: Expansion of a few selected images from the expanded dataset.

Demonstration: eigencat

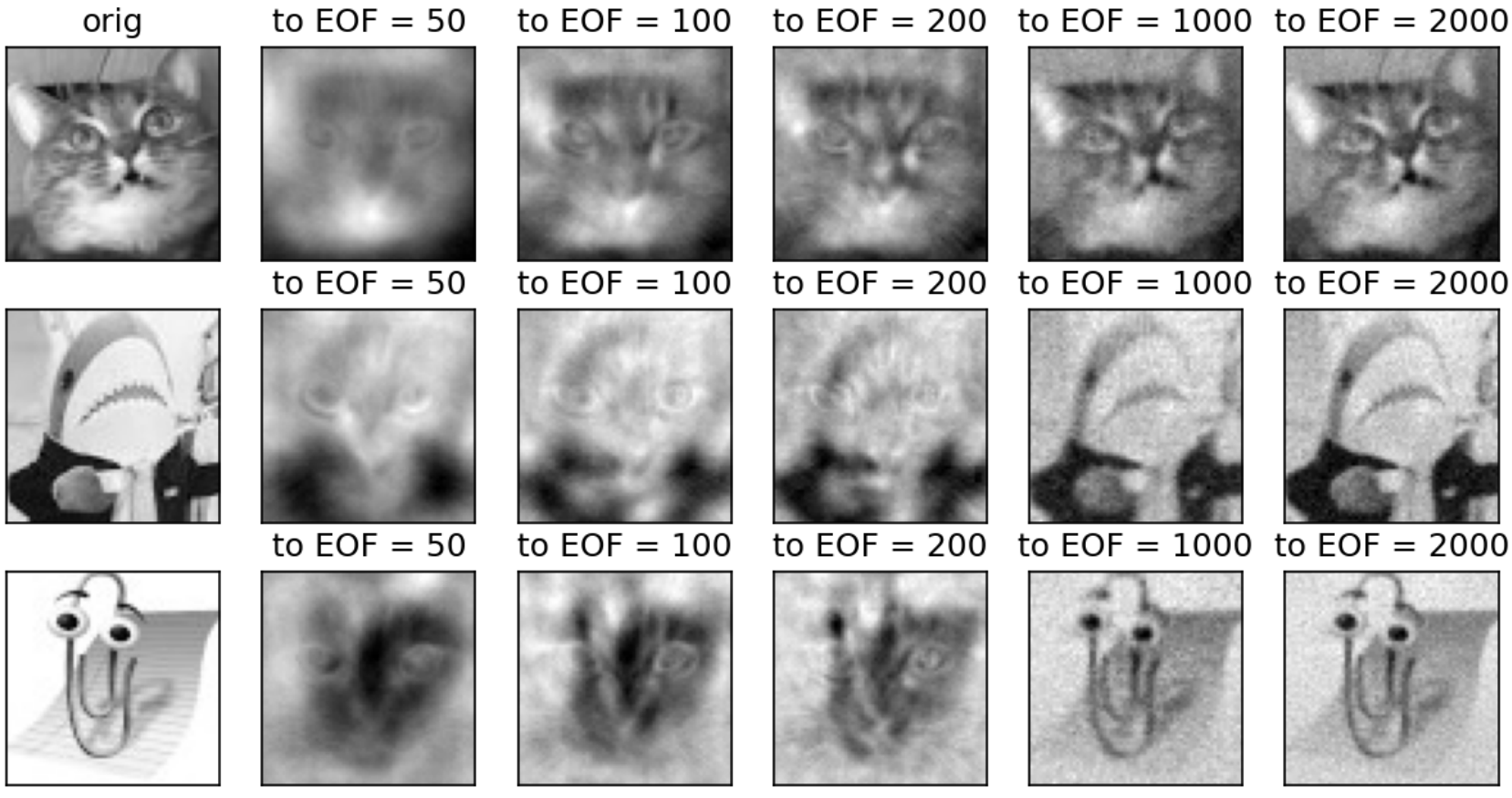


Figure: Eigencat expansion of the three ad hoc TAs (which were not in the dataset).

Clustering: a motivation

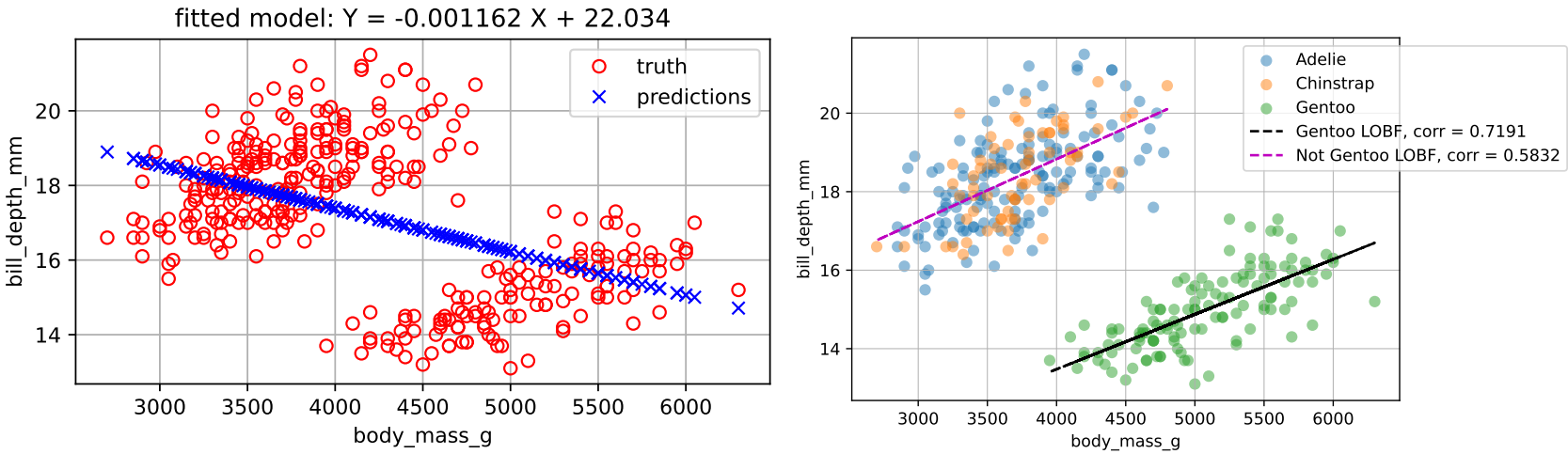


Figure: Contrived example of completely different models depending on data selection.

- if we had no labels in penguins data the linear regression is pretty bad (although it was never going to be good...)

  $\rightarrow$ use clustering to create labels?

  $\rightarrow$ e.g. use that to inform training of model, or to train different models

Oceanographic examples

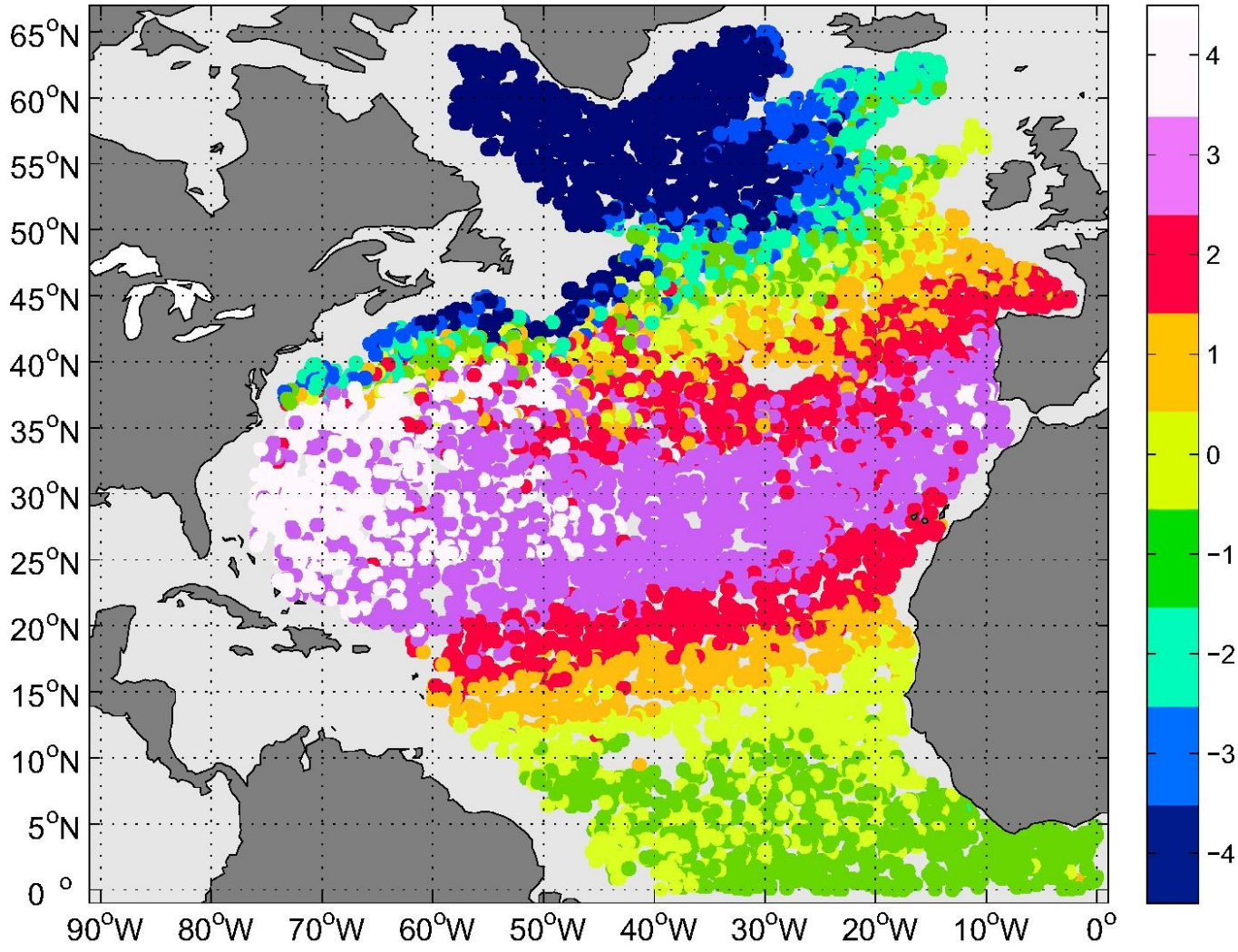


Figure: From Maze *et al.* (2017), Fig. 4. Gaussian Mixture Model to identify watermass clusters from Argo data in Atlantic.

Oceanographic examples

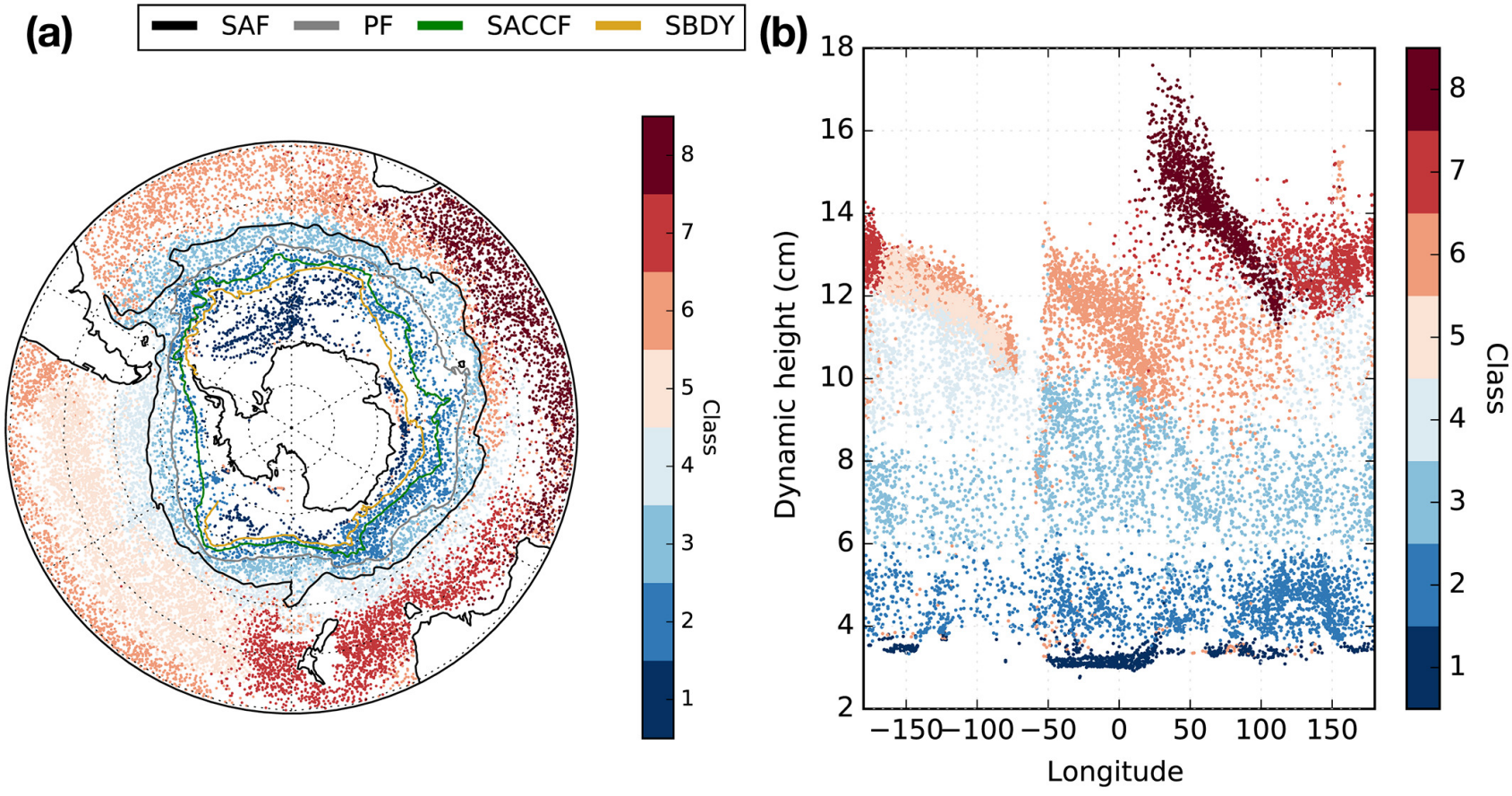


Figure: From Jones *et al.* (2019), Fig. 5. Gaussian Mixture Model to identify watermass clusters from Argo data in Southern Ocean.

Oceanographic examples

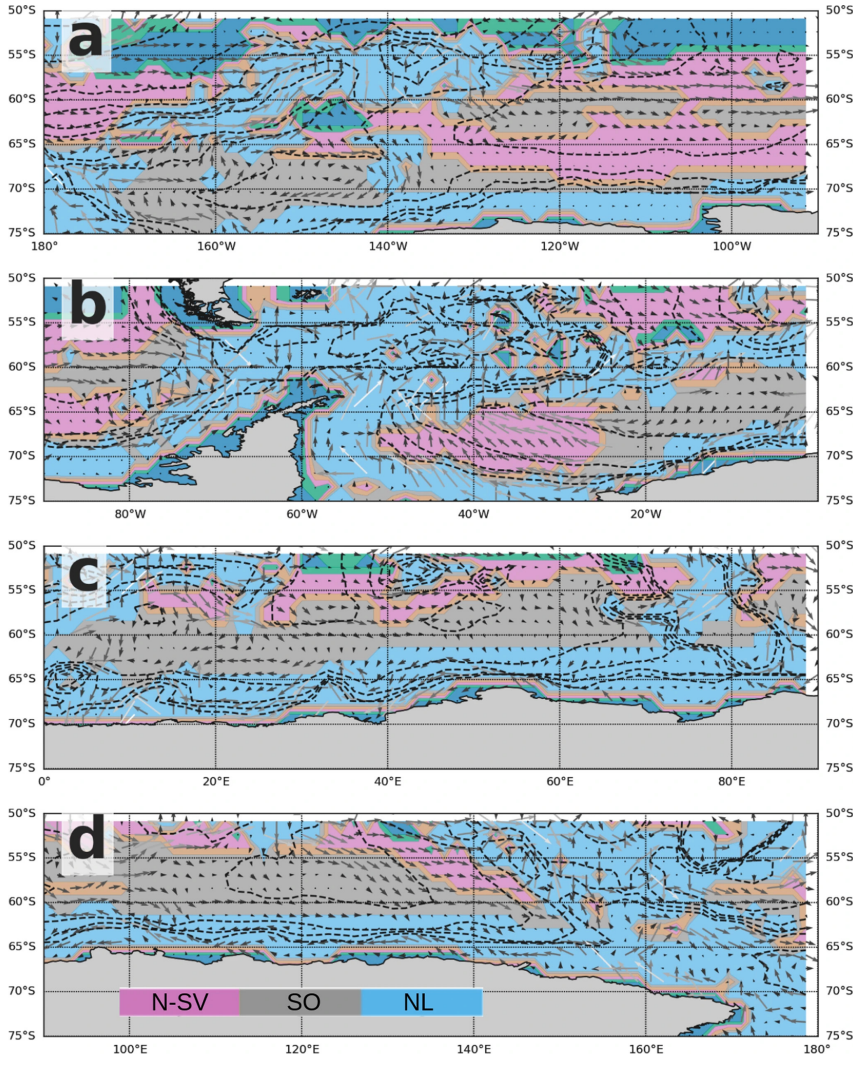


Figure: From Sonnewald *et al.* (2023), Fig. 4. *k*-means to identify clusters based on dynamic (from barotropic vorticity budget).

Oceanographic examples

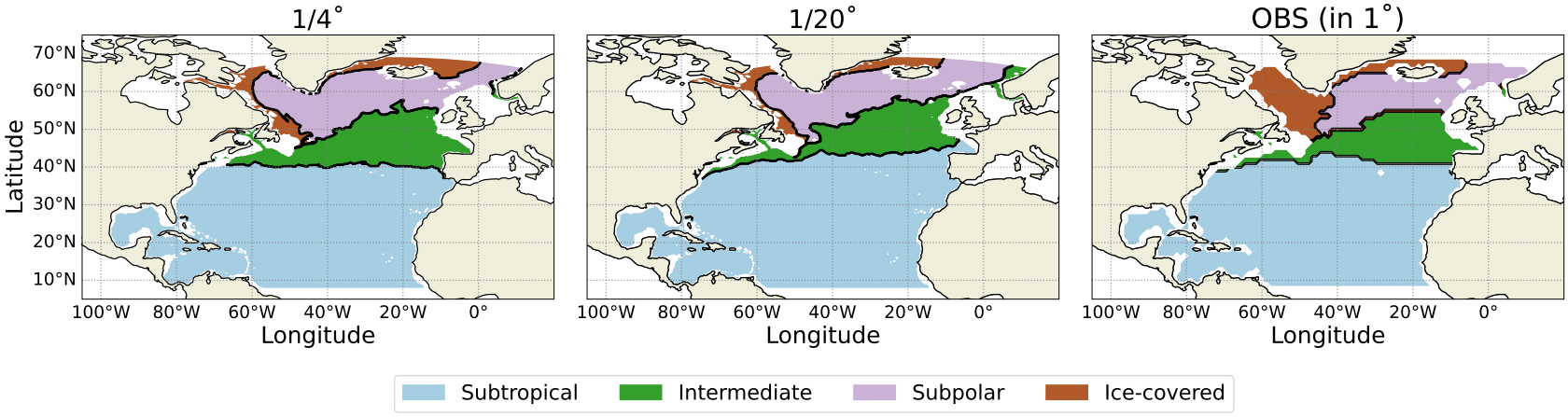


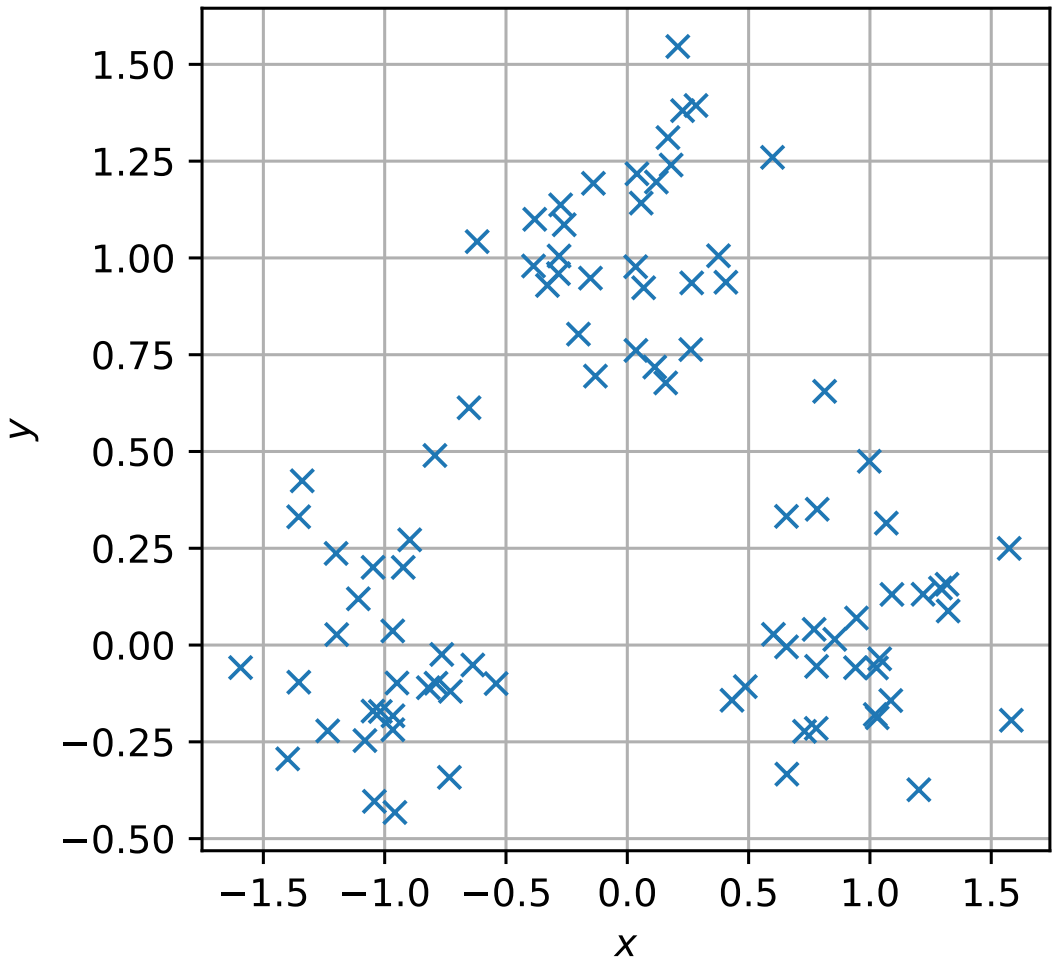
Figure: From Ruan *et al.* (in prep.), which identifies regions depending on biogeochemical activity.

- hierachy building of clusters using various variables
  → SST, MLD, sea-ice fraction, not (lon, lat)
  → nitrate concentation, surface chlorophyll concentration

- aim to classify POC and DOC export, but do not include those in building of cluster

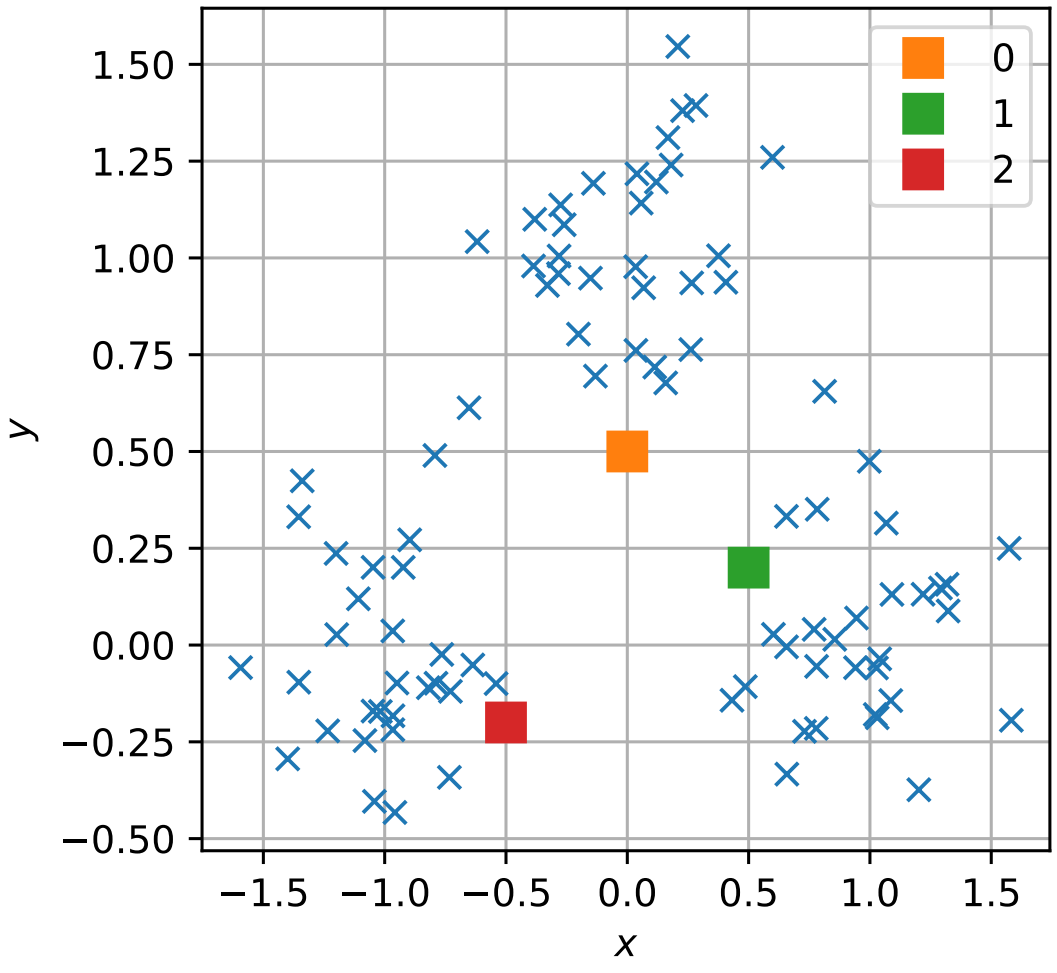
e.g. K-means

- demonstrate the algorithm with K-means
  $\rightarrow$ artificially create some data ($K = 3$ is sensible)



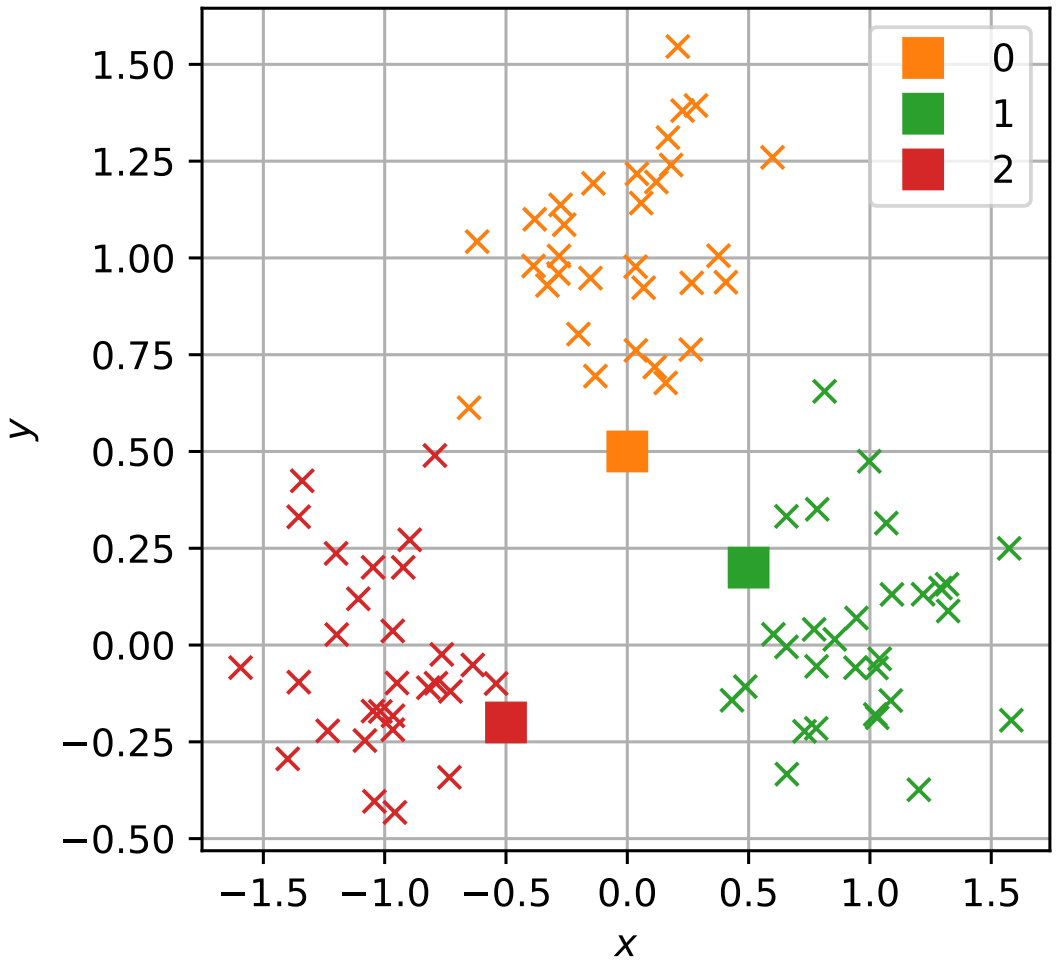
e.g. K-means

- provide initial centres of clusters
  $\rightarrow$ K-means is quite robust, can just guess



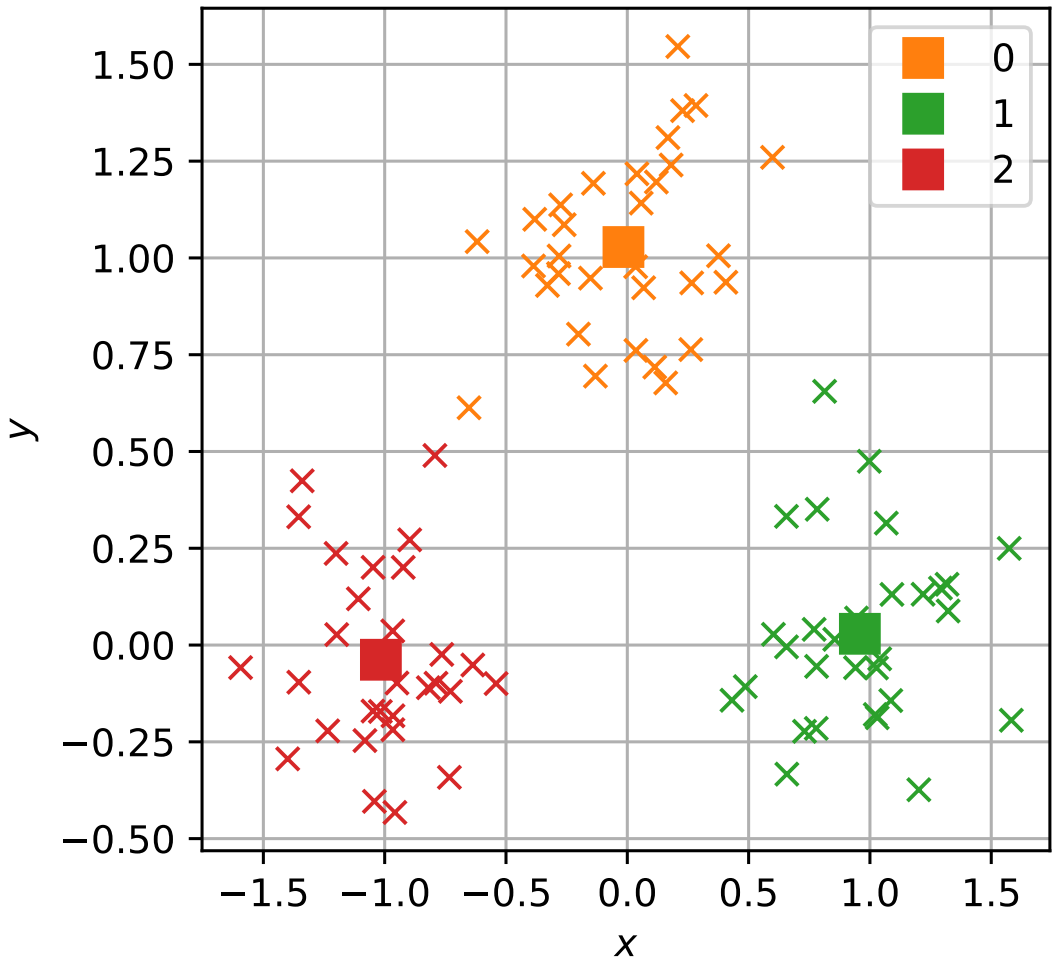
e.g. K-means

- label points closest to centres accordingly
  $\rightarrow$ distance dependent, normally L^2 (Euclidean distance)



e.g. K-means

- from new cluster, find the new location of the centre
  $\rightarrow$ update and iterate accordingly



K-means in `sklearn`

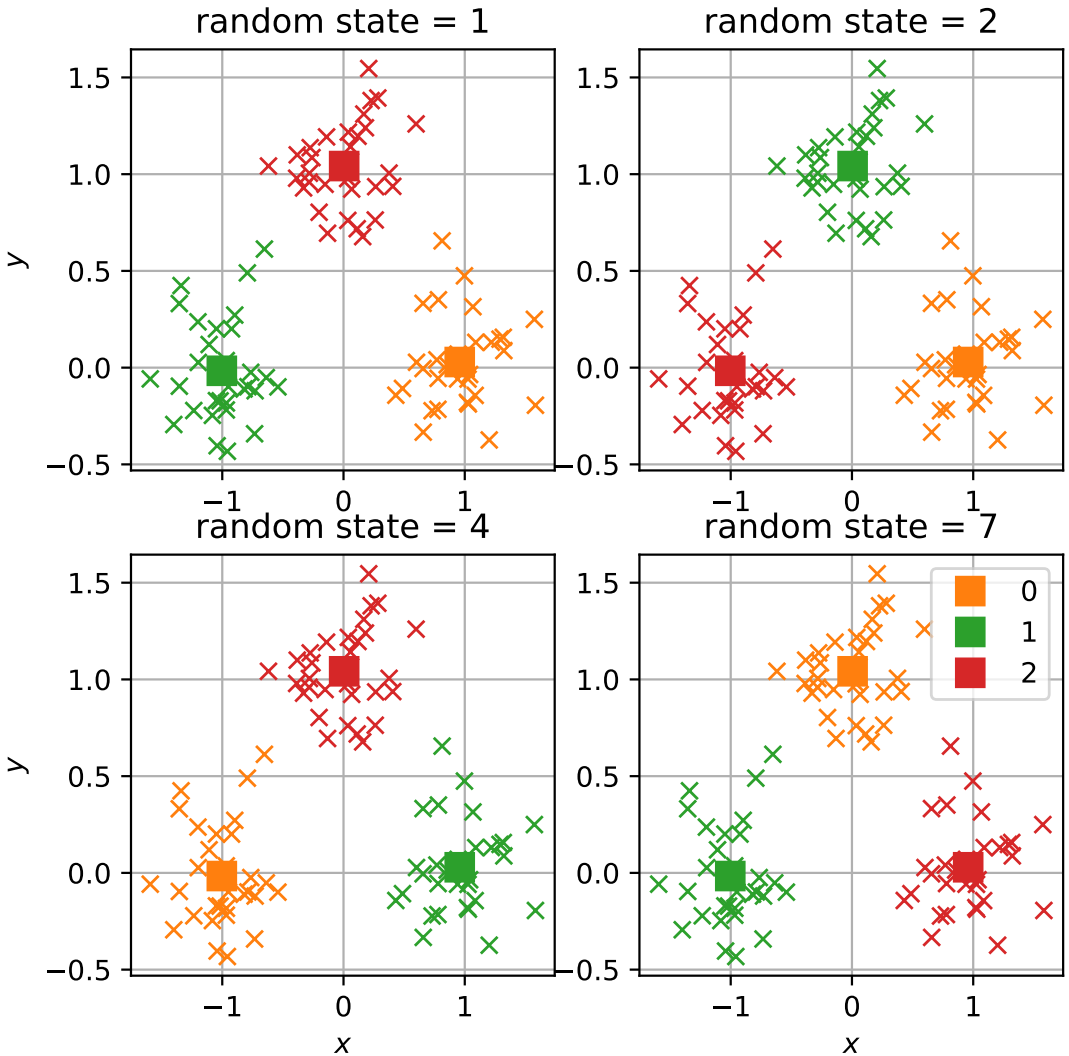


Figure: *K*-means through `sklearn`. Random state changes initial guess.

A case where K-means as is will never(?) work

- all of the above depends on the choice of 'distance' again

A case where K-means as is will never(?) work

- all of the above depends on the choice of 'distance' again
- there are well-known examples where the L^2 distance is simply not the relevant one
  $\rightarrow$ e.g. the moon data (2d example) and Swiss roll data (can do 2d or 3d)

Figure: Moon Moon and two rolled up towels resembling a Swiss roll.

A case where K-means as is will never(?) work

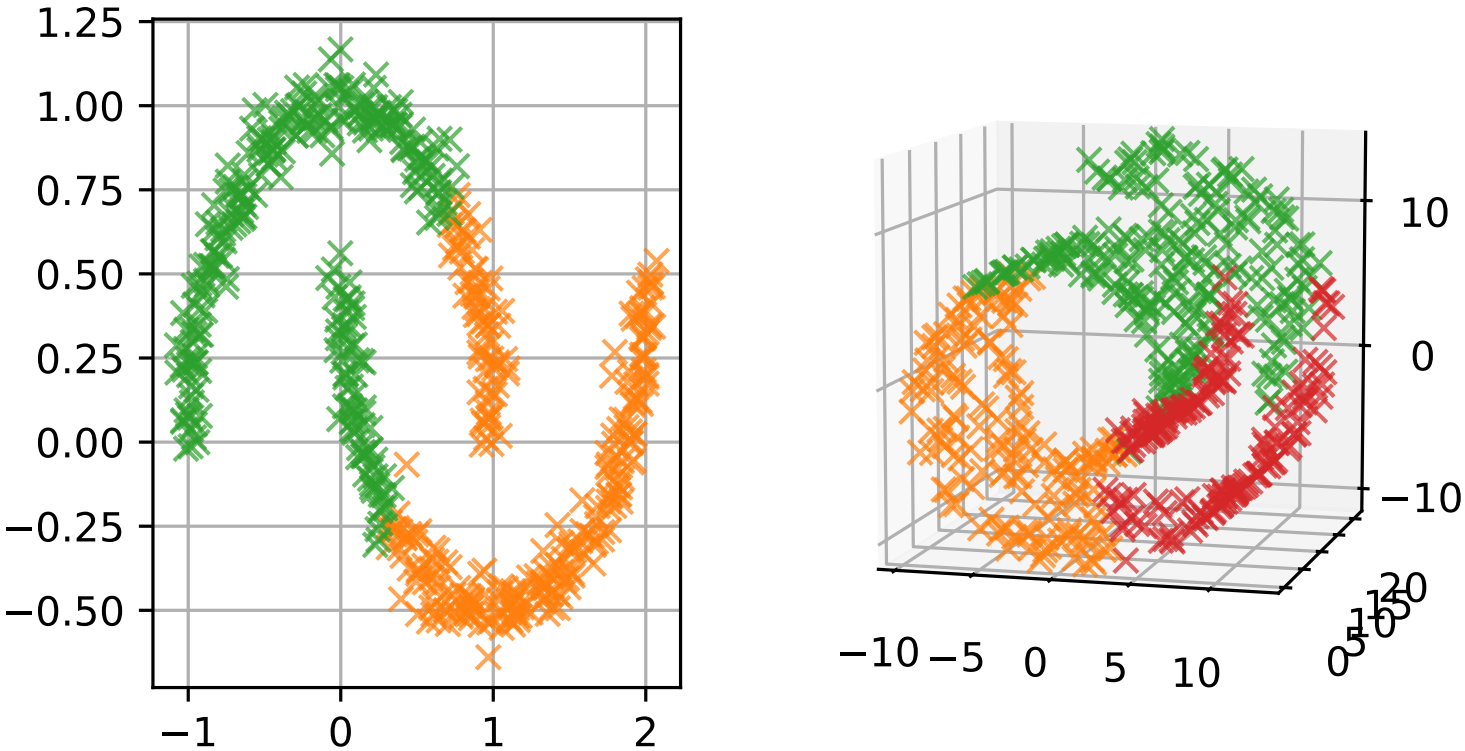


Figure: K-mean as applied to the crescent moons and swiss roll data.

The issue of 'distance'

- the data may have structure and lives on a curve/surface/volume etc. (e.g. manifold up to noise)

  $\rightarrow$ manifold may have a lower dimension structure (1d and 2d here)

  $\rightarrow$ but embedded in an ambient space ($\mathbb{R}^2$ and $\mathbb{R}^3$ here)

The issue of 'distance'

- the data may have structure and lives on a curve/surface/volume etc. (e.g. manifold up to noise)

  $\rightarrow$ manifold may have a lower dimension structure (1d and 2d here)

  $\rightarrow$ but embedded in an ambient space ($\mathbb{R}^2$ and $\mathbb{R}^3$ here)
- it is the distance intrinsic to the manifold that is presumably of interest

  $\rightarrow$ L^2 is the distance extrinsic to manifold and inherited from the ambient/embedding

- find a suitable embedding, as in dimension reduction previously?

  $\rightarrow$ reduce dimension first, then cluster

Moon data demonstration

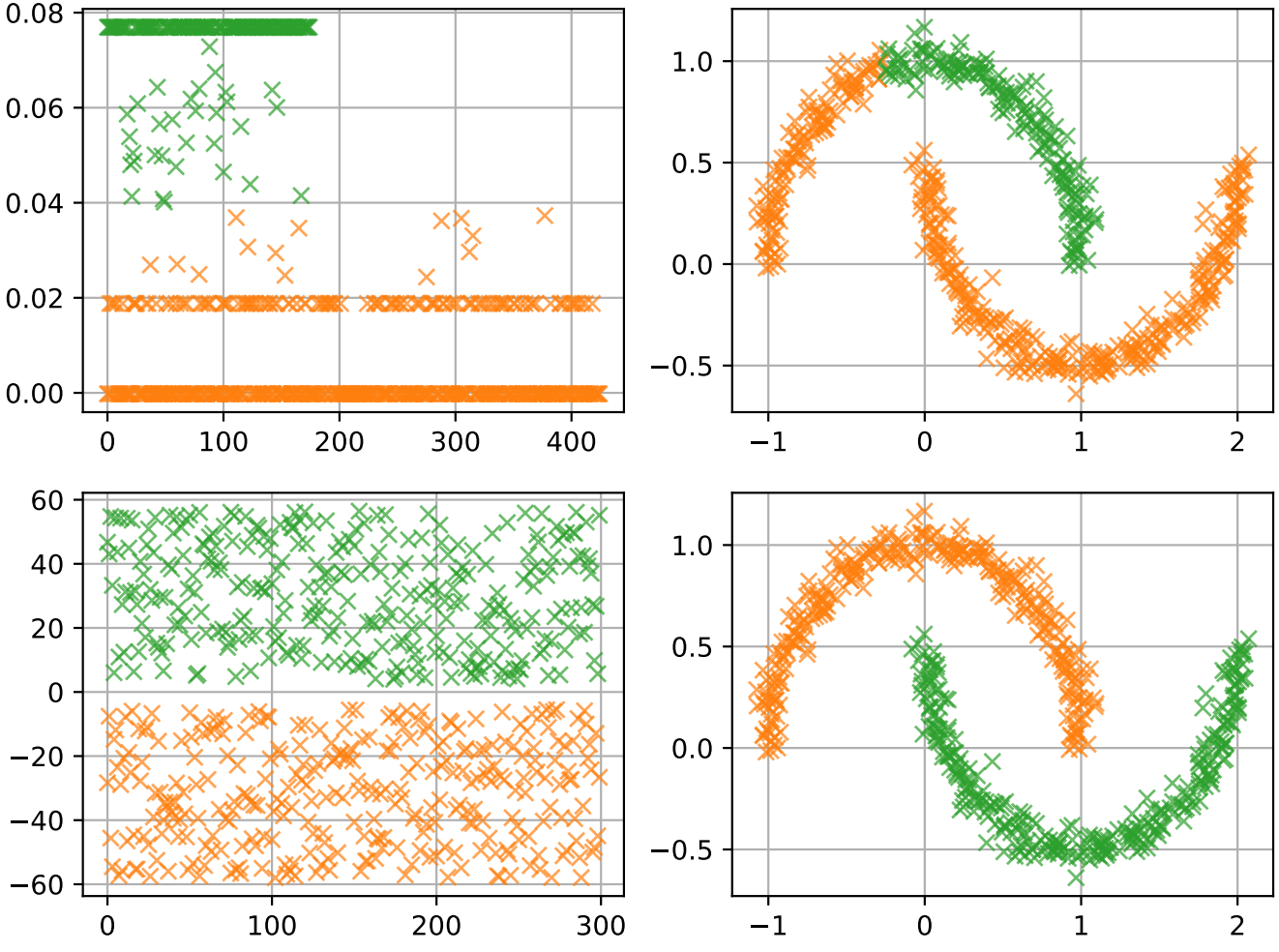


Figure: 1d projection (of 2d data) via (top) LLE and (bottom) *t*-SNE before *K*-means. LLE can work on occasions, but *t*-SNE seems more robust.

Swiss roll data demonstration

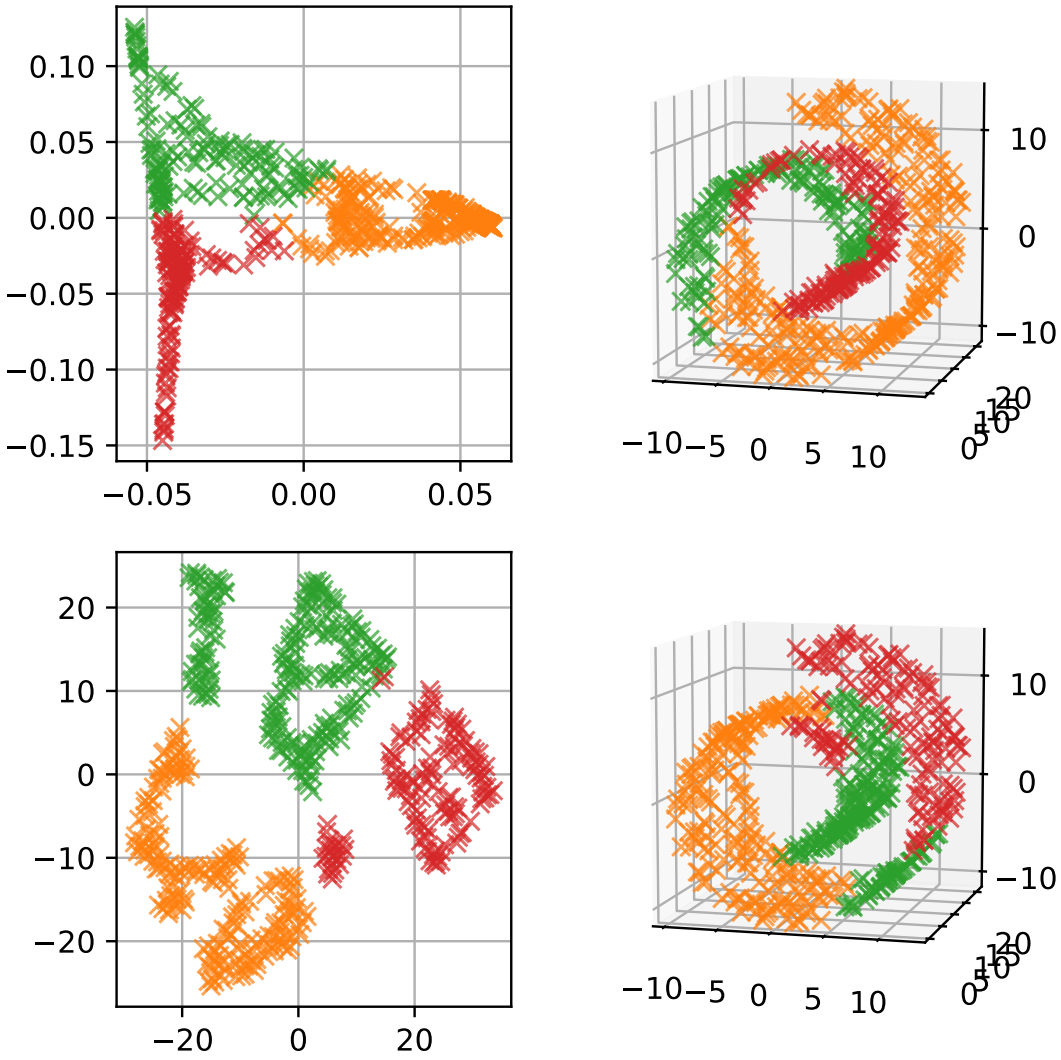


Figure: 2d projection (of 3d data) via (top) LLE and (bottom) t-SNE before K-means. LLE arguably segments better.

Other algorithms (e.g. DBSCAN)

- other algorithms do things differently
- DBSCAN considers clusters as high density regions and gaps are low density regions

  $\rightarrow$ two parameters: radius ϵ of some ball and number of points within said ball to quantify 'density'

  $\rightarrow$ number of clusters identified is a result of the above two choices (unlike in K-means)

  $\rightarrow$ can deal with non-Euclidean distances (you need to provide it though)

- hyper-parameter tuning + cross-validation needed!

Other algorithms (e.g. DBSCAN)

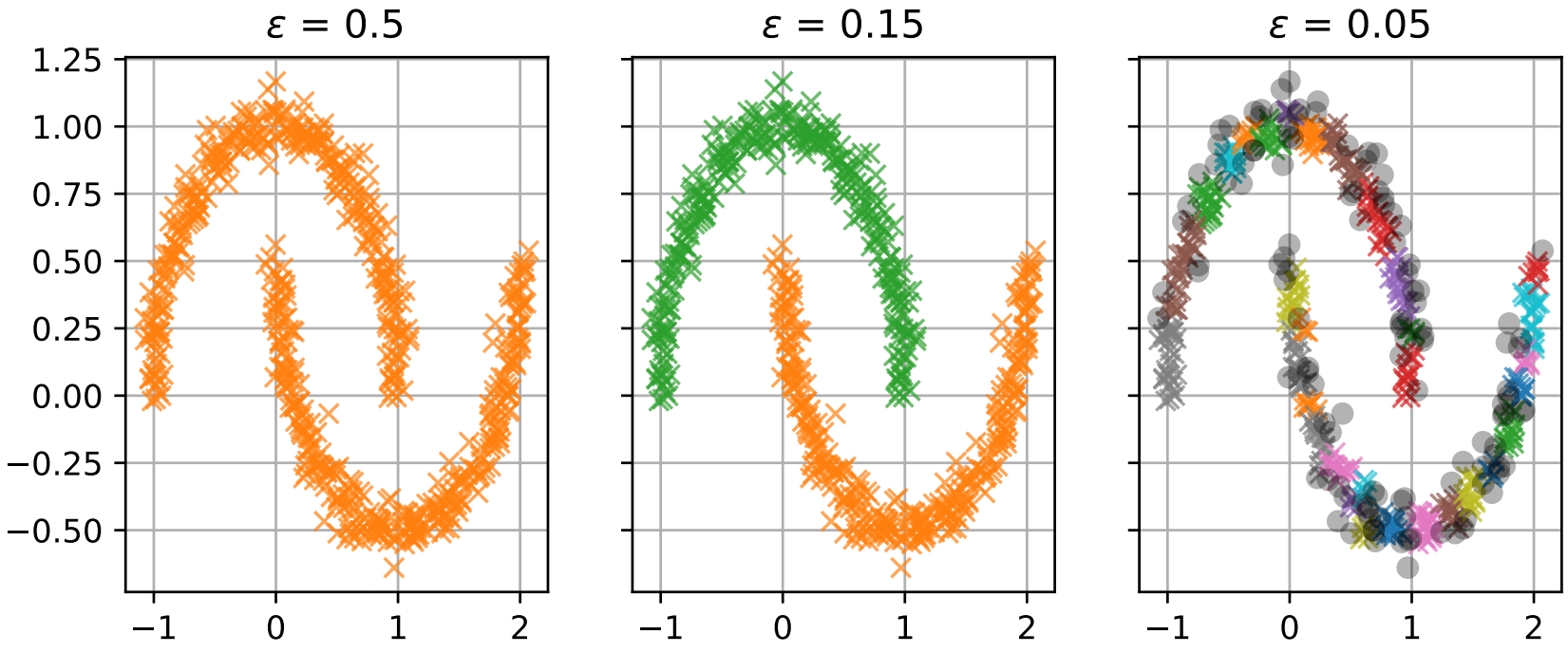


Figure: DBSCAN on moon data at varying ϵ.

- optimal ϵ for the two clusters
- if too small the too many clusters identified

  $\rightarrow$ black points are 'noise' points (no confidence in which cluster it should fall in)

Other algorithms (e.g. DBSCAN)

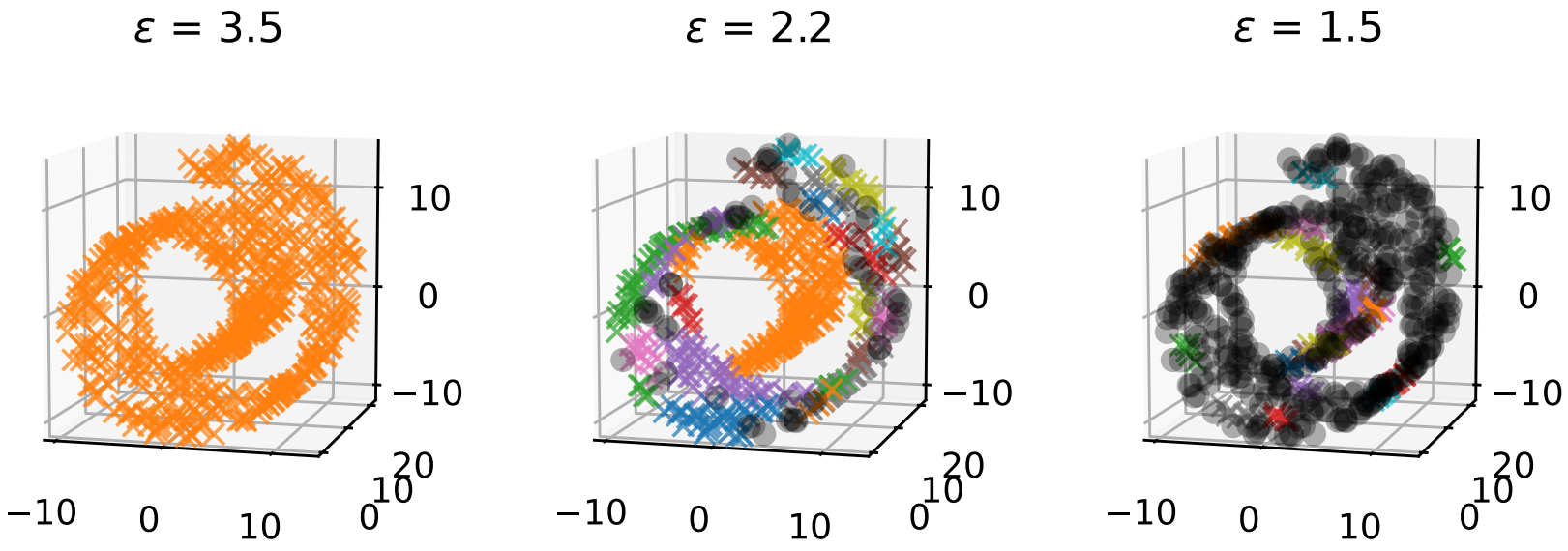


Figure: DBSCAN on swiss roll data at varying ϵ.

- optimal ϵ for the one giant cluster (bit contrived though...)
- smaller ϵ leads to segmenting along the surface, so ok

Demonstration: penguins data

- K-means ($K = 3$) on full 4d data (standardised per feature), then compare classification skill
  $\rightarrow$ some manual remapping needed
  $\rightarrow$ skill is around 91% accuracy for this realisation

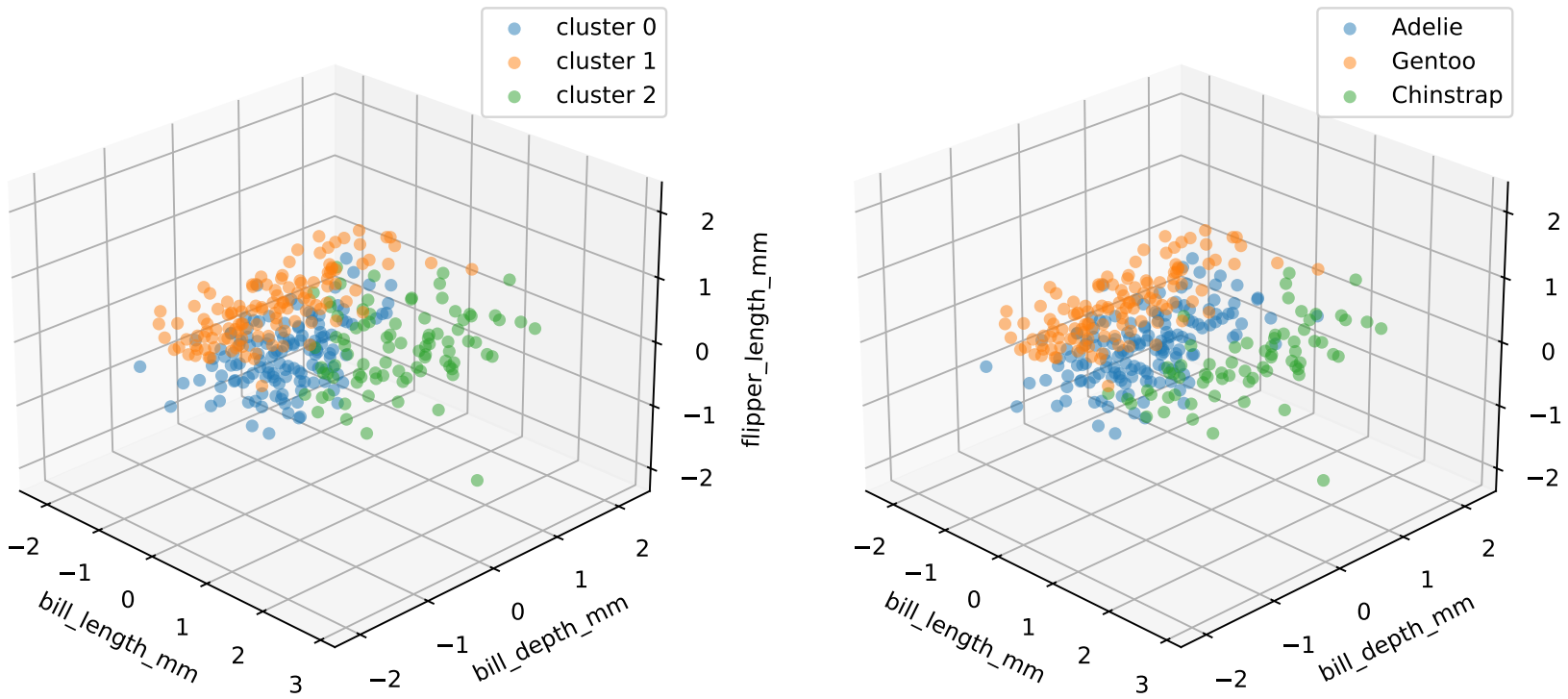


Figure: K-means on standardised penguins data.

Demonstration: penguins data

- as above but with a t-SNE to 2d before K-means

  $\rightarrow$ some manual remapping needed

  $\rightarrow$ skill is around 96% accuracy for this realisation

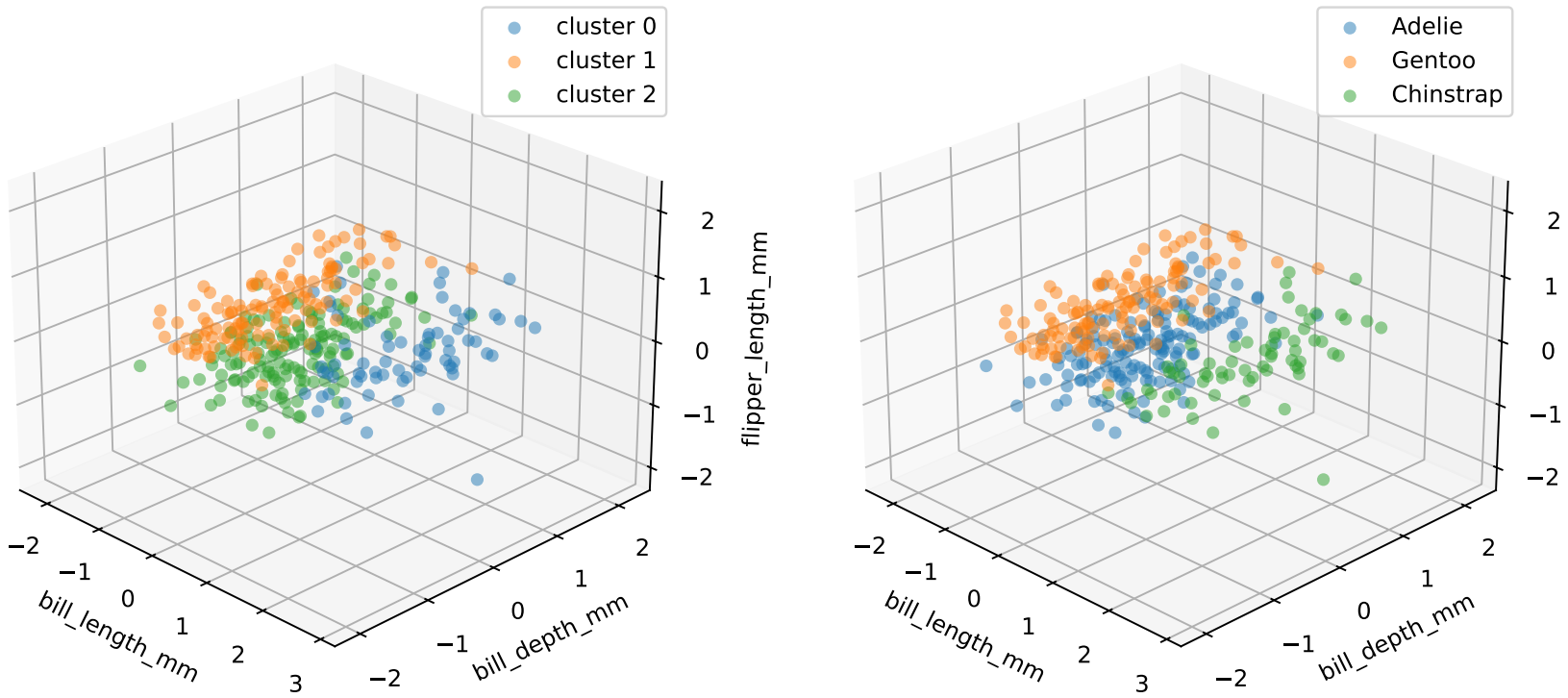


Figure: t-SNE to 2d before K-means on standardised penguins data.

Validation and model robustness

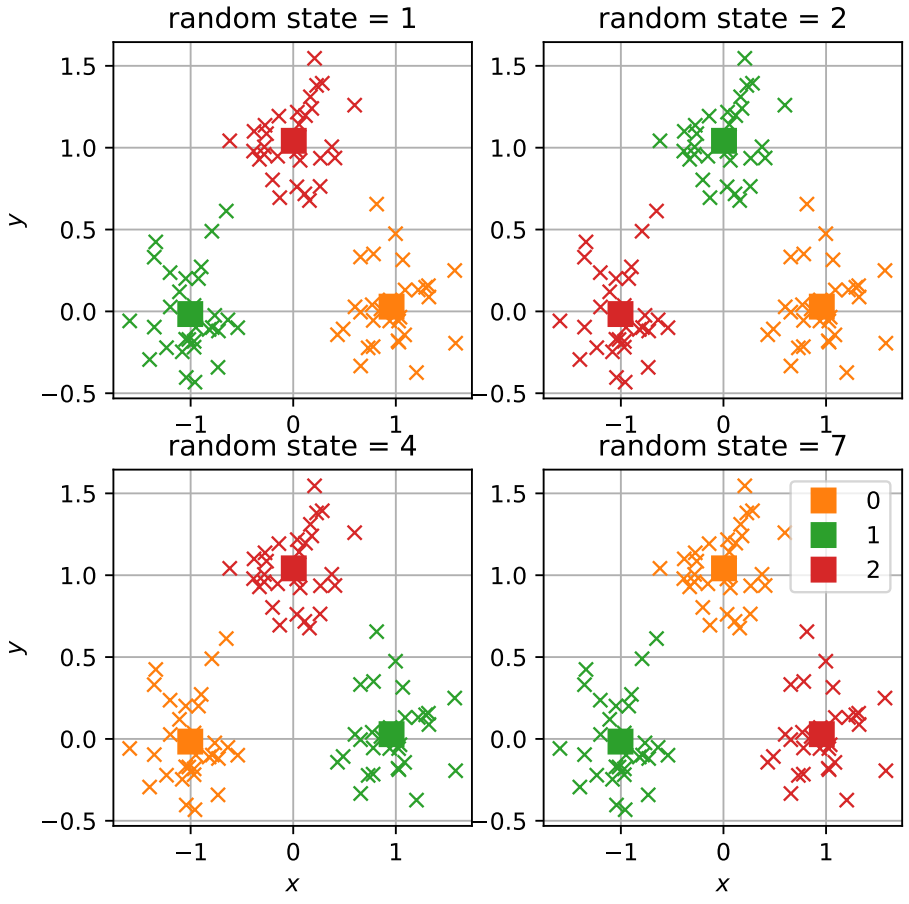


Figure: *K*-means through `sklearn`. Random state changes initial guess.

- there is inherent randomness in the training

  → e.g. from train-test split

  → resulting models can have some randomness also

  → how do we know our model 'works' not just because we got 'lucky'?

Validation and model robustness

- just do what we would normally do with statistics, e.g.
  $\rightarrow$ train an ensemble and take some averages
  $\rightarrow$ evaluate sensitivity to choices made
  $\rightarrow$ quantifying/probing for uncertainties
  $\rightarrow$ evaluate on possible over-fitting
  $\rightarrow$ ...

what you wouldn't do with statistics
you should not do with machine learning

Cross-validation

- over-fitting is when model has skill in training, but may suck in test case

  $\rightarrow$ particularly if testing data is outside the pdf of the training data
- e.g. high degree polynomial fitting

$$\hat{Y} = \sum_{i=0}^{p} a_i X^i = a_0 + a_1 X^1 + a_2 X^2 + \ldots$$

  $\rightarrow$ the degree of polynomial p could be regarded as the model hyperparameter here

  $\rightarrow$ blows up quickly outside of training range

- probably best to regarded most ML models as over-fitted unless shown otherwise...

e.g., k-fold cross validation

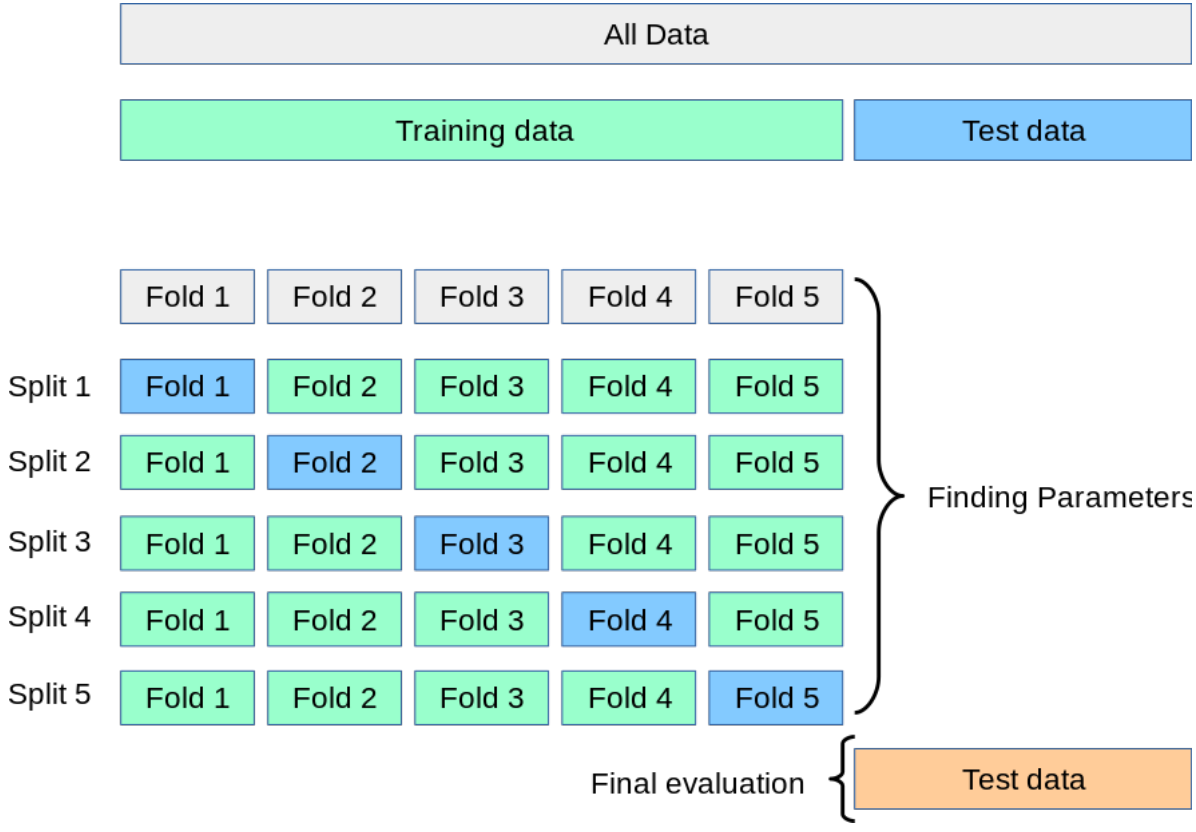


Figure: Schematic of k-fold cross-validation. Taken from `https://scikit-learn.org/stable/modules/cross_validation.html`.

- do repeated training on the folds, then do testing
  $\rightarrow$ the training thus also serve as validation set

Cross-validation

- then select 'best' model, e.g.

  $\rightarrow$ select best choice of p

  $\rightarrow$ select the $\{a_i\}$ that performs best during training

  $\rightarrow$ average the $(a_0, a_1, \ldots)$ and use the "averaged" model

  $\rightarrow \ldots$

- similarly if having a whole load of different models

  $\rightarrow$ for linear models next lecture, do the above but for linear regression, LASSO, ridge, etc.

Demonstration

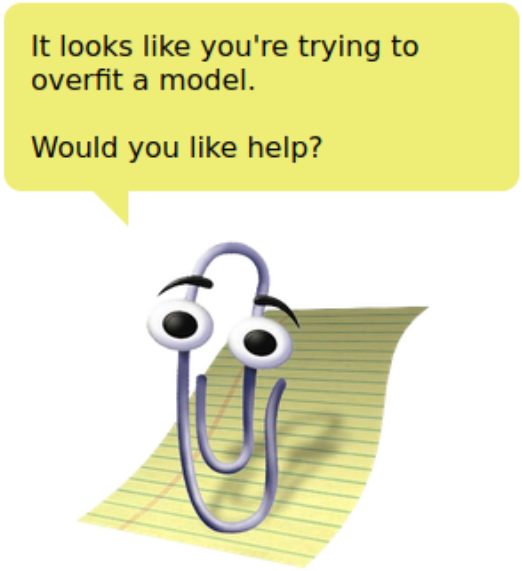


Figure: The OG AI (which was mega annoying by the way).

- (deterministic) linear models as variations of the loss function
- examples of dimensional reduction and feature identifications
- clustering as a way to create features
- need for hyper-parameter tuning and model validation

what you wouldn't do with statistics
you should not do with machine learning

Moving to a Jupyter notebook →