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  `https://github.com/julianmak/OCES4303_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 4303 :

an introduction to data-driven and ML methods in ocean sciences

Session 3: some linear models and dimension reduction

Outline

- some linear models
  → Linear Regression, Ridge, Lasso, Elastic-Net
  → gradient descent to obtain model

  (avoiding probability based ones somewhat)

- dimension reduction
  → PCAs, locally linear embedding, t-SNE

- demonstration: eigencat

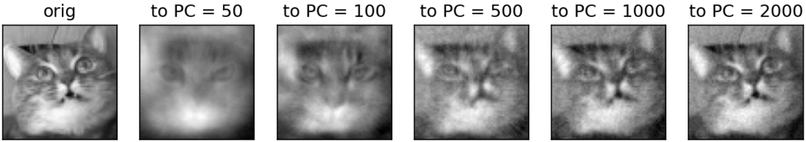

Figure: Result from an eigencat projection (it's really just PCAs).

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)

  $\rightarrow$ these were termed **multi**-linear models in OCES 3301

- 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 αs 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

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

$\rightarrow$ ρ is a ratio hyper-parameter controlling sparsity and model parameter values **(cross-validation needed!!)**

Sample loss function + gradient descent

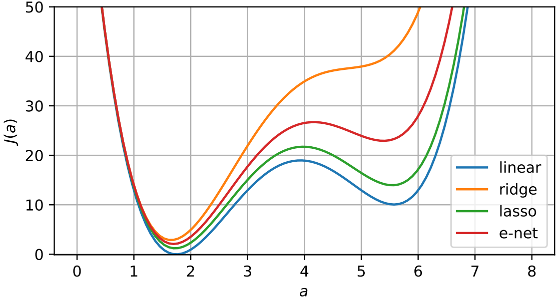

Figure: Made up 1d example of $J = J(a)$ with different choices of regularisation, $J = (1/2M)\|\hat{Y} - Y\|_{L^2}^2 + \alpha\rho\|a\|_{L^1} + (1/2)\alpha(1-\rho)\|a\|_{L^2}^2$.

- 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

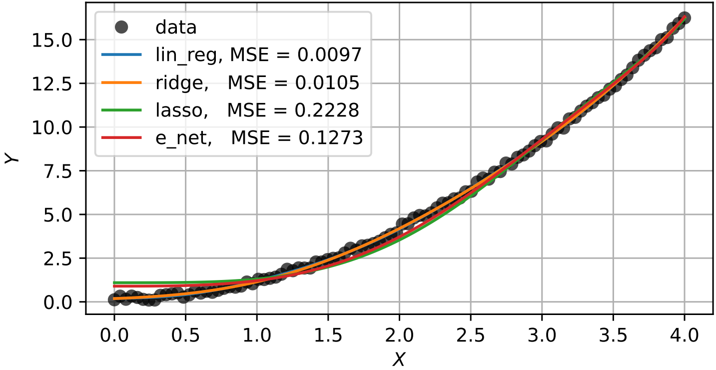

Figure: Polynomial regression for some contrived data, with MSE scores printed on.

Example: regressing to polynomial data

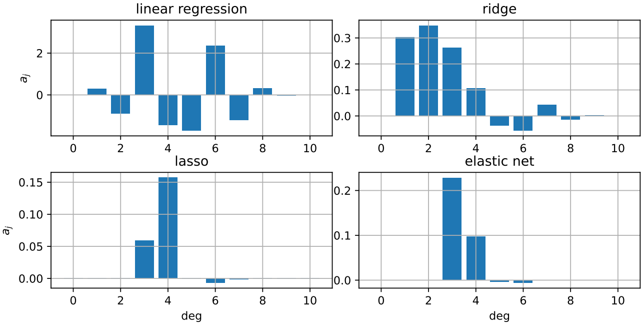

Figure: Polynomial regression for some contrived data, with MSE scores printed on.

- 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?)

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

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- Principal Component Analysis (PCA) is one way

  $\rightarrow$ seen already from OCES 3301

  $\rightarrow$ 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 visually with the penguins example maybe
  $\rightarrow$ data has been standardised here

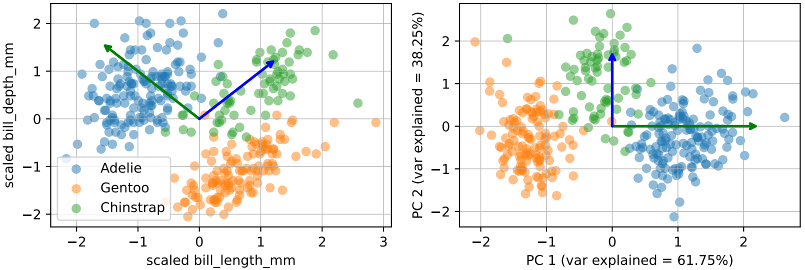


Figure: (Left) Original (but standarised) data with two choices of variables. (Right) The same but in the principal component representation.

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

Dimension reduction: PCAs

- below shows dimension reduction (from 4 to 2)

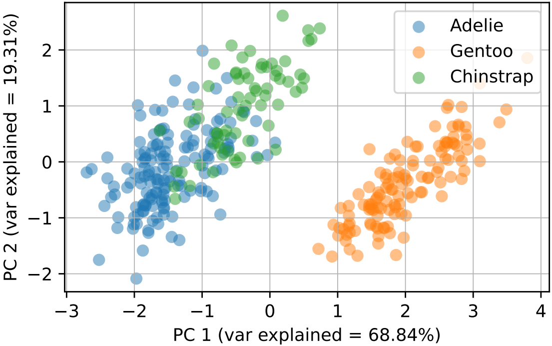


Figure: Representation in PC1 and PC2 co-ordinate system.

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

Dimension reduction: manifold methods

(This part makes more sense after next session)

- 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)

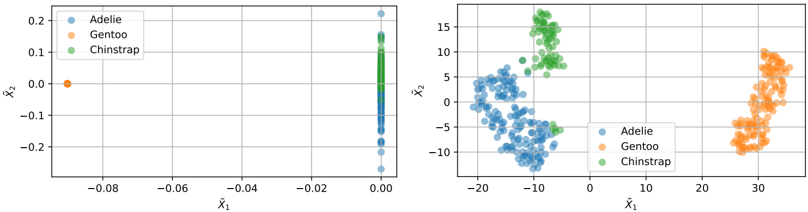


Figure: Demonstration of Locally Linear Embedding and *t*-SNE on the penguins data.

Demonstration: eigencat

- example demonstrating PCA on images of cats

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

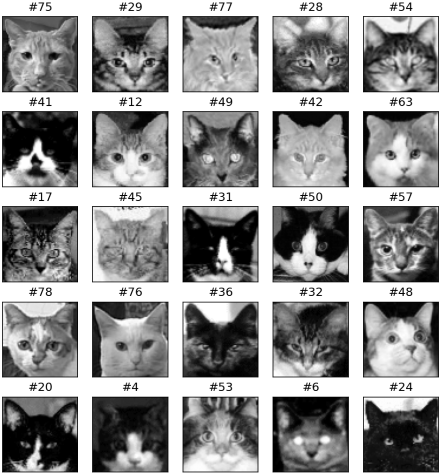


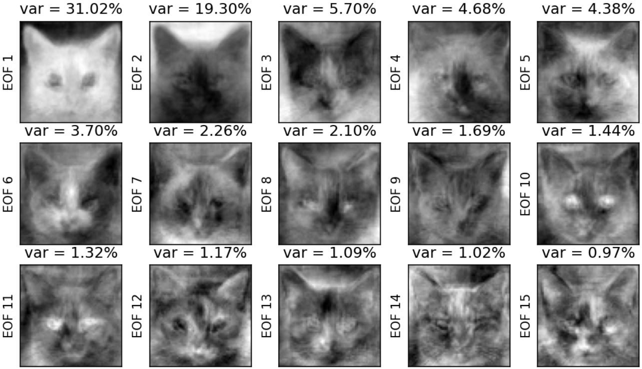
Figure: Data in `cats.csv`.

Demonstration: eigencat

- want

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

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



Demonstration: eigencat

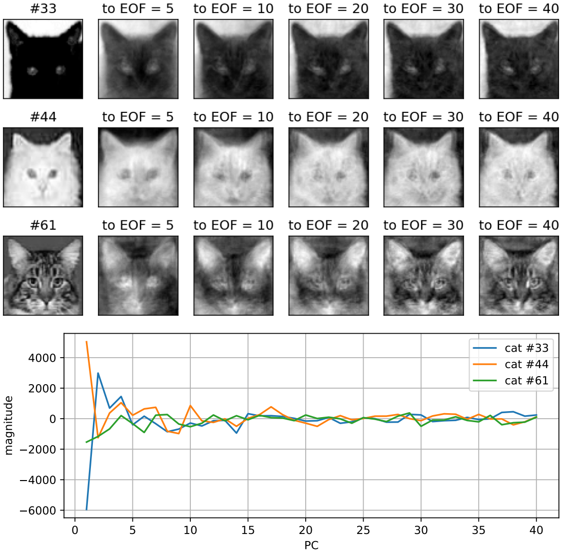


Figure: Expansion and loadings of three of the samples.

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

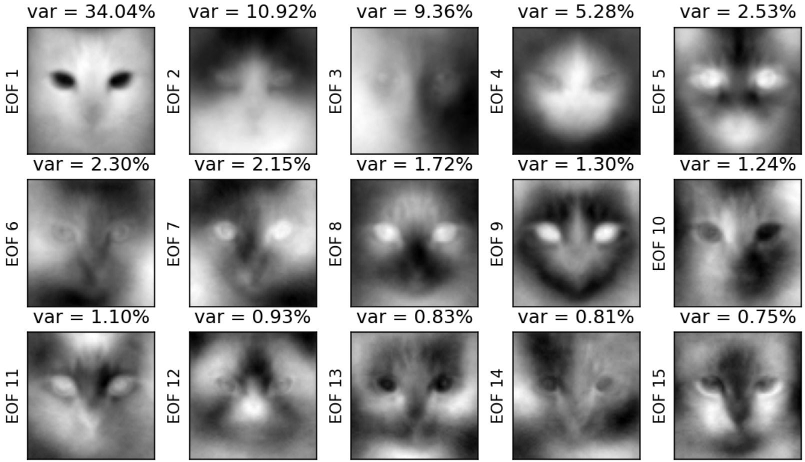


Figure: Eigencats from `cats_bw_enlarged.csv`.

Demonstration: eigencat

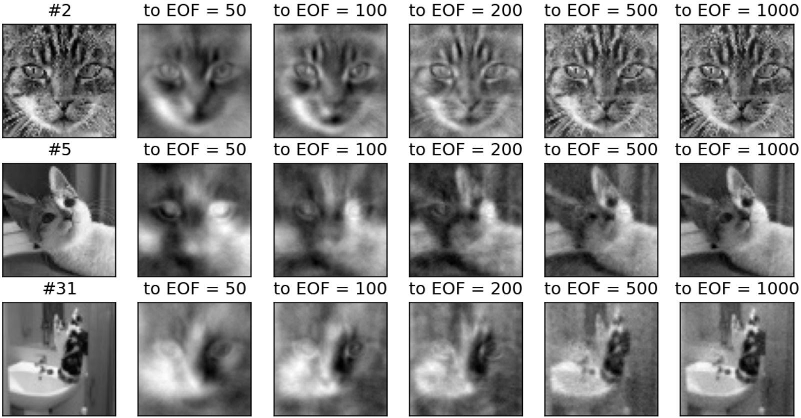


Figure: Expansion of a few selected images from the expanded dataset.

Demonstration: eigencat

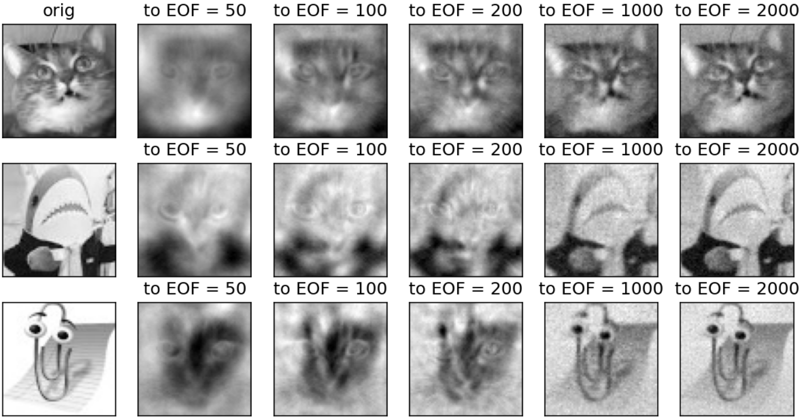


Figure: Eigencat expansion of the three ad hoc TAs (which were not in the dataset).

Demonstration

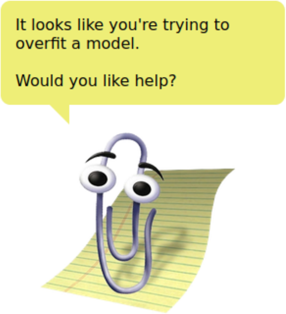


Figure: The OG AI (which was mega annoying by the way).

- demonstrating some linear models

  $\rightarrow$ avoided probability based linear models (see notebook for references)
- basics and extended example of dimensional reduction and feature identifications

Moving to a Jupyter notebook $\rightarrow$