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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 5: classifications

Outline

- classification

  → predicting **discrete** labels (cf. **continuous** target in regression)

  → e.g. predicting species, image classification, etc.

- task of finding a separators between data

  → Linear/Quadratic Discrimnant Analysis (L/QDA)

  → Support Vector Machine (SVM)

  → general choices of loss function + regularisation through Stochastic Gradient Descent (SGD)

  → digression: links with neural networks later

- demonstration: penguins data

Example: predicting label from data

- suppose I have the following data:

bill length (mm)	55.0
bill depth (mm)	20.0
flipper length (mm)	207.0
body mass (g)	4000.0

Q. what is the associated species of penguin?

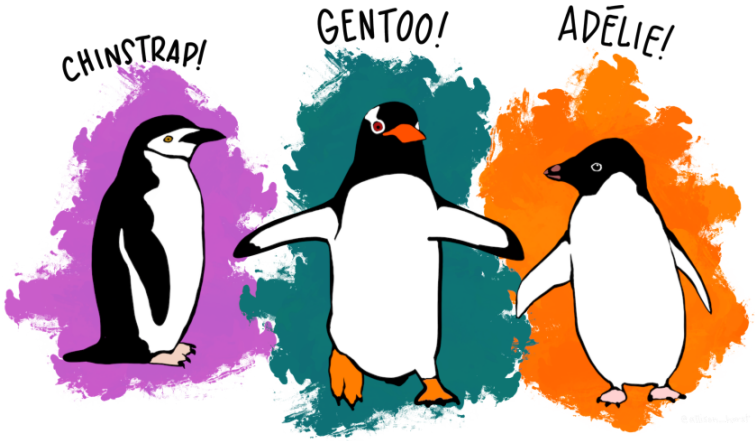


Figure: Palmer penguins logo. From `https://allisonhorst.github.io/palmerpenguins/`

Example: image classification

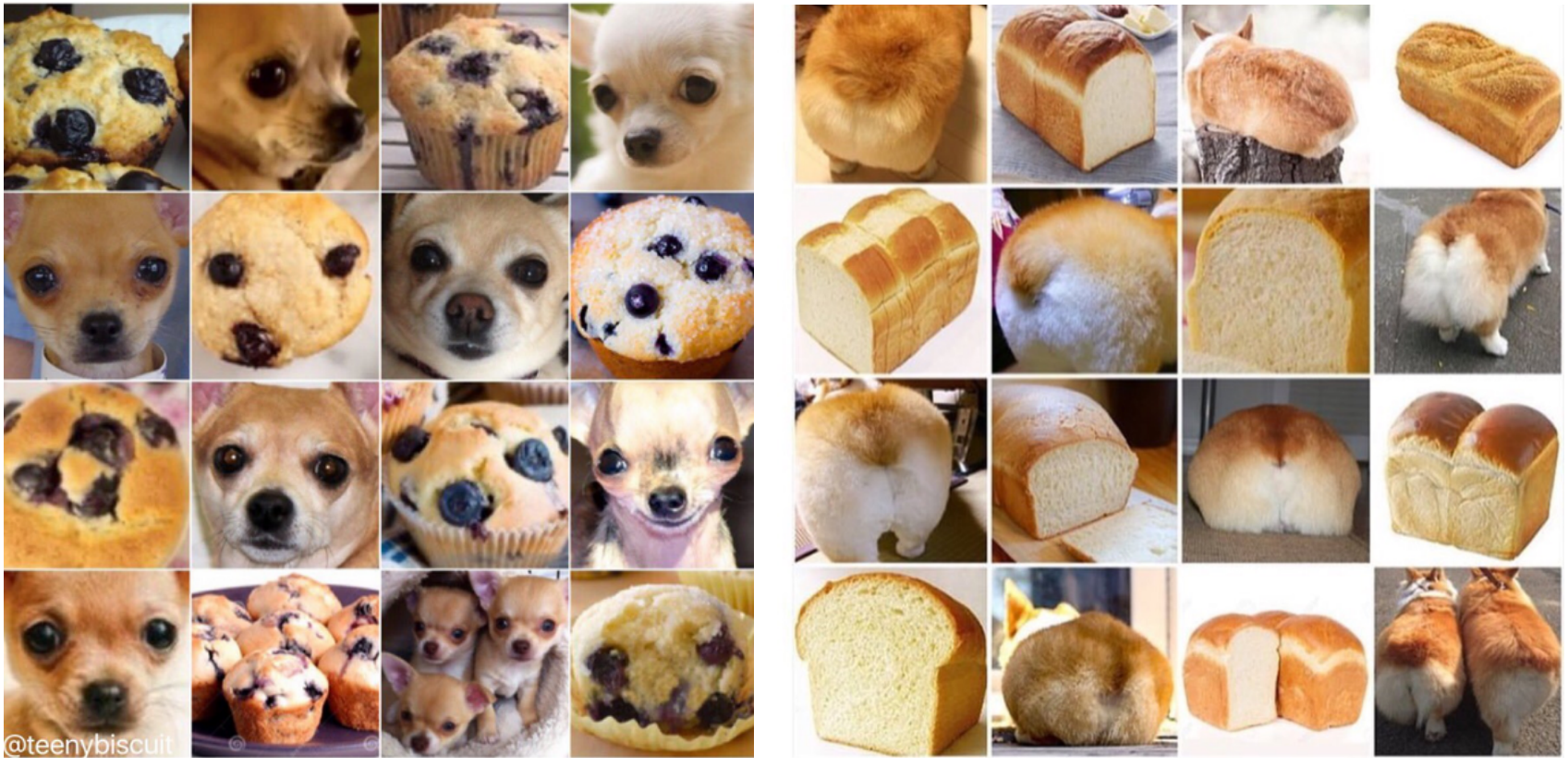


Figure: Various entries from the "animal or things" meme, as found on the internet.

Classification as a geometry problem

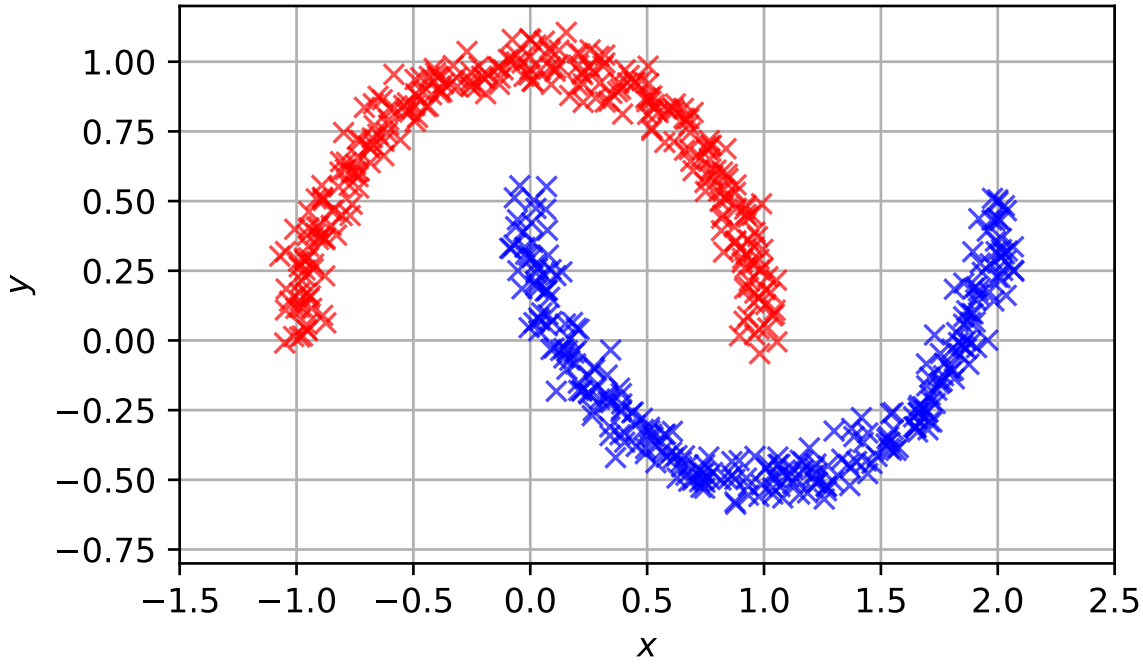


Figure: Moon data coloured by the cluster it is in.

- moon data as an example
- task: find the line/curve that separates the data clusters

  → a separator (there are many of these)

  → higher dimension analog: (hyper-)planes/surfaces

L/QDA

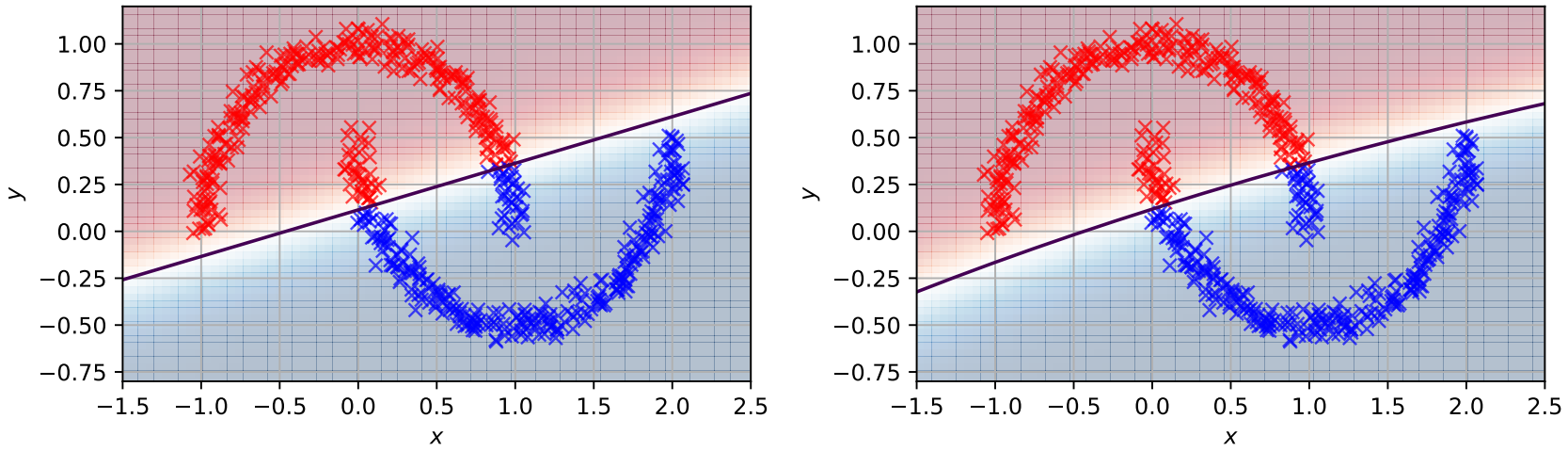
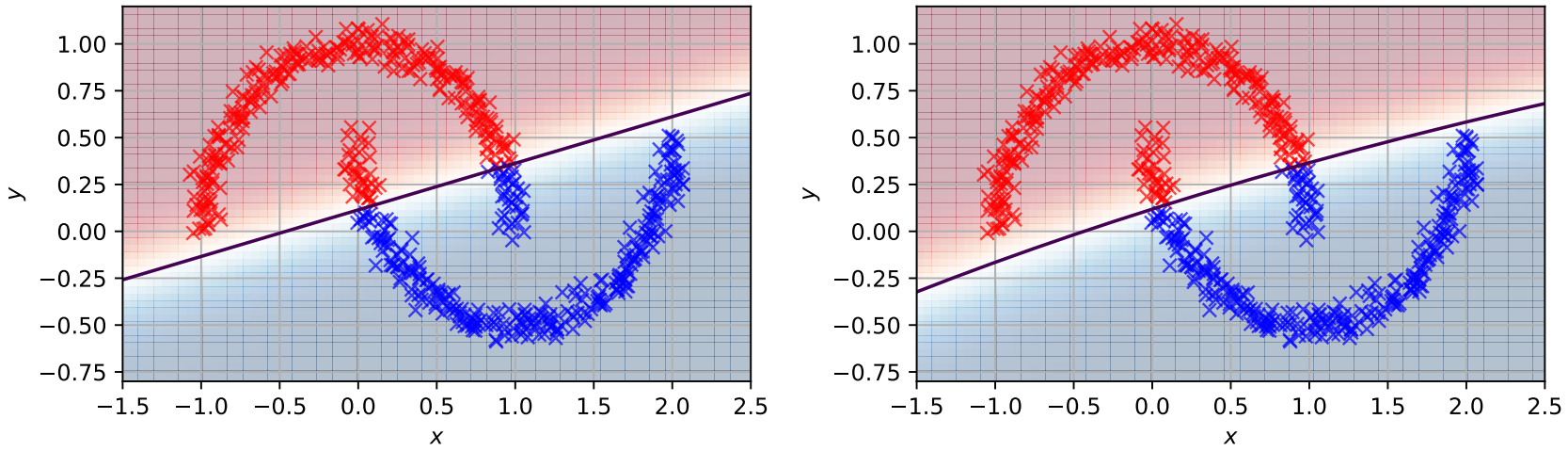


Figure: Classification by a realisation of (left) LDA and (right) QDA, with decision boundaries and probabilities.

- Linear/Quadratic Discriminant Analysis (L/QDA)
  → finds a linear/quadratic separator
  → closed form solutions, quite robust
  → an approach related to statistics, has probability measures associated with this (the shading)

L/QDA



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Q. more complex curve needed?

SVM

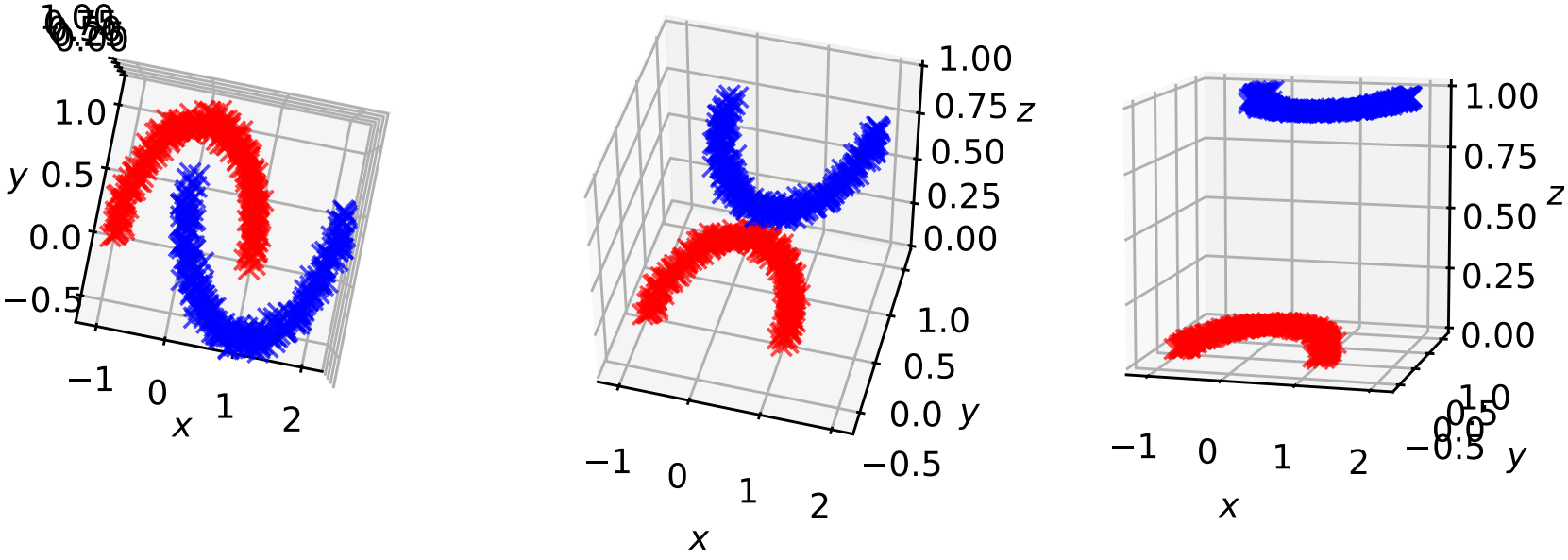

Figure: Moon data where I artificially 'lift' one of the clusters.

- instead of more complex curve, what about simpler separator but 'lift' the data instead to a higher dimension?

  $\rightarrow$ basic geometric idea of Support Vector Machine (SVM)

SVM

- with enough complexity the data can almost always be separable

  $\rightarrow$ then easy to find separating hyper-plane

  $\rightarrow$ can arbitrarily find complicated dimension promotions though?

  $\rightarrow$ mapping can be expensive computationally?

SVM

- with enough complexity the data can almost always be separable

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  $\rightarrow$ can arbitrarily find complicated dimension promotions though?

  $\rightarrow$ mapping can be expensive computationally?

- idea: find **maximal** hyper-plane separator given a remapping into higher-dimensions, but **penalise** the complexity of that transformation

  $\rightarrow$ an optimisation problem

(actually uses the kernel trick and solving the dual problem; not going to elaborate on those)

SVM

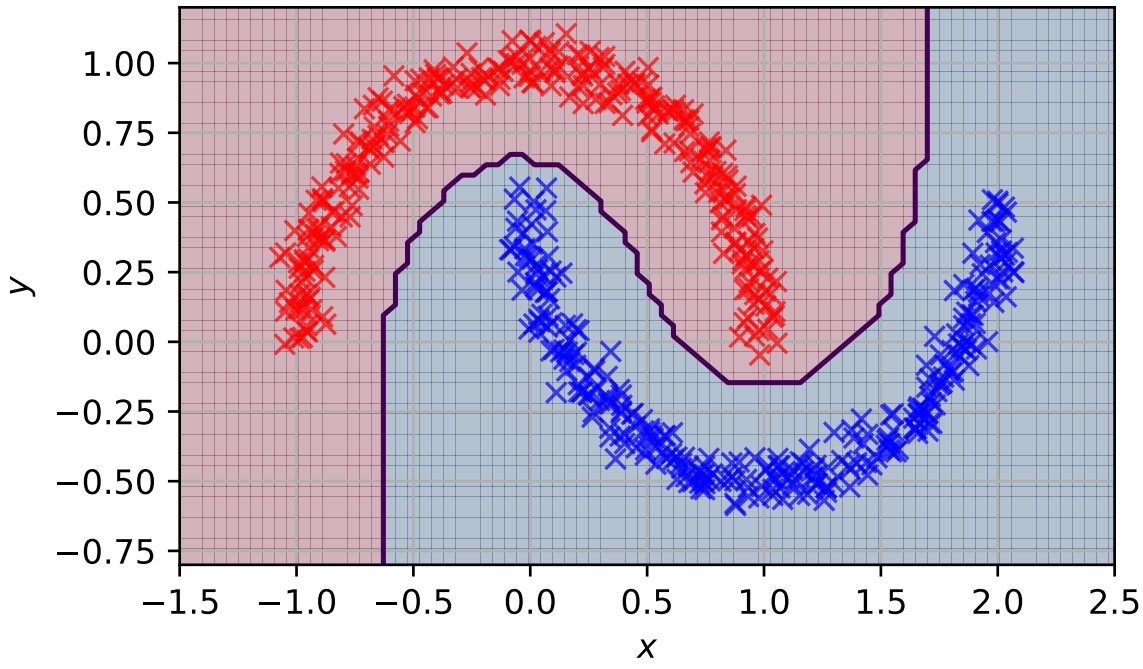

Figure: Moon data using a SVM with the radial basis function as the kernel.

- roughly: transform data, find hyper-plane, undo transformation

  $\rightarrow$ no probability measure here for decision

SVM

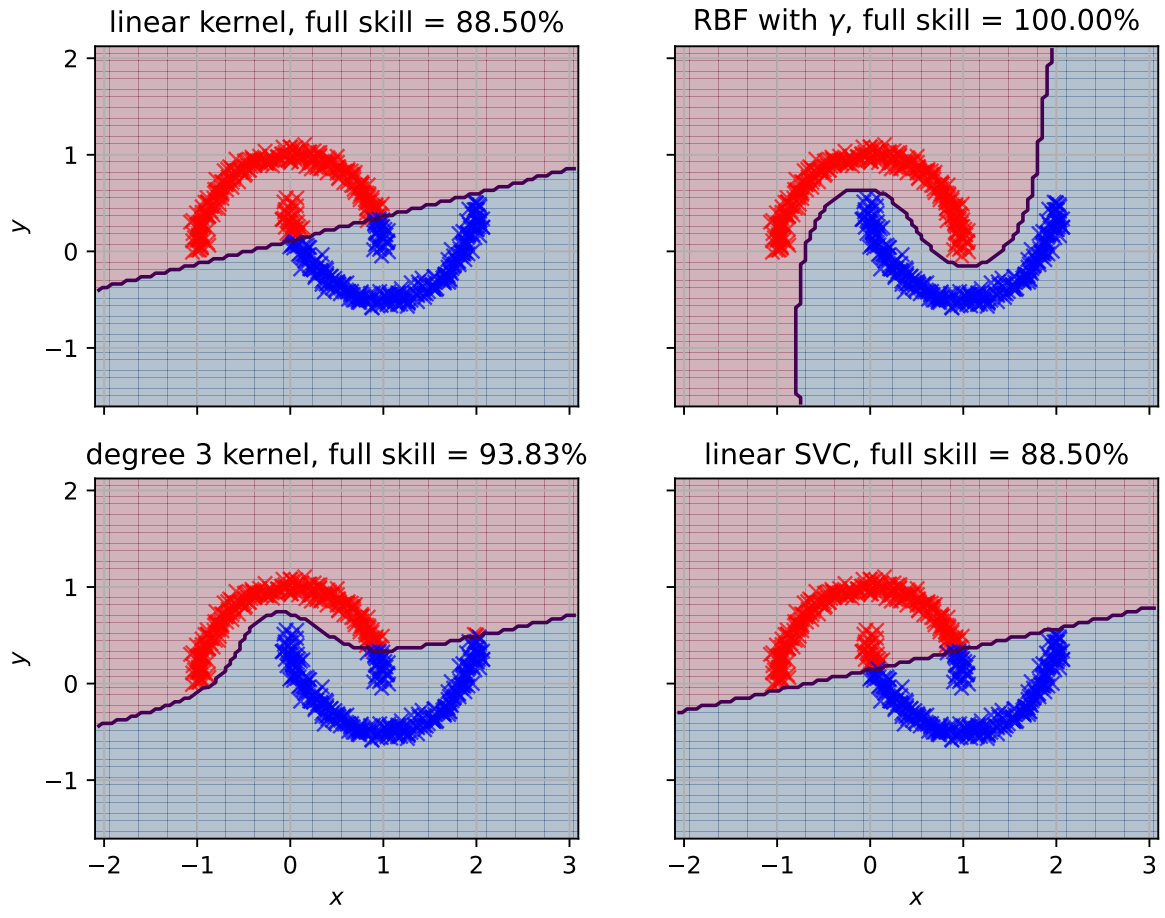

Figure: SVM on moon data with different choices of kernels and regularisations.

Issues with SVM: dependence on scaling

- SVM not invariant to re-scaling
  $\rightarrow$ highly recommended to scale/standardise data

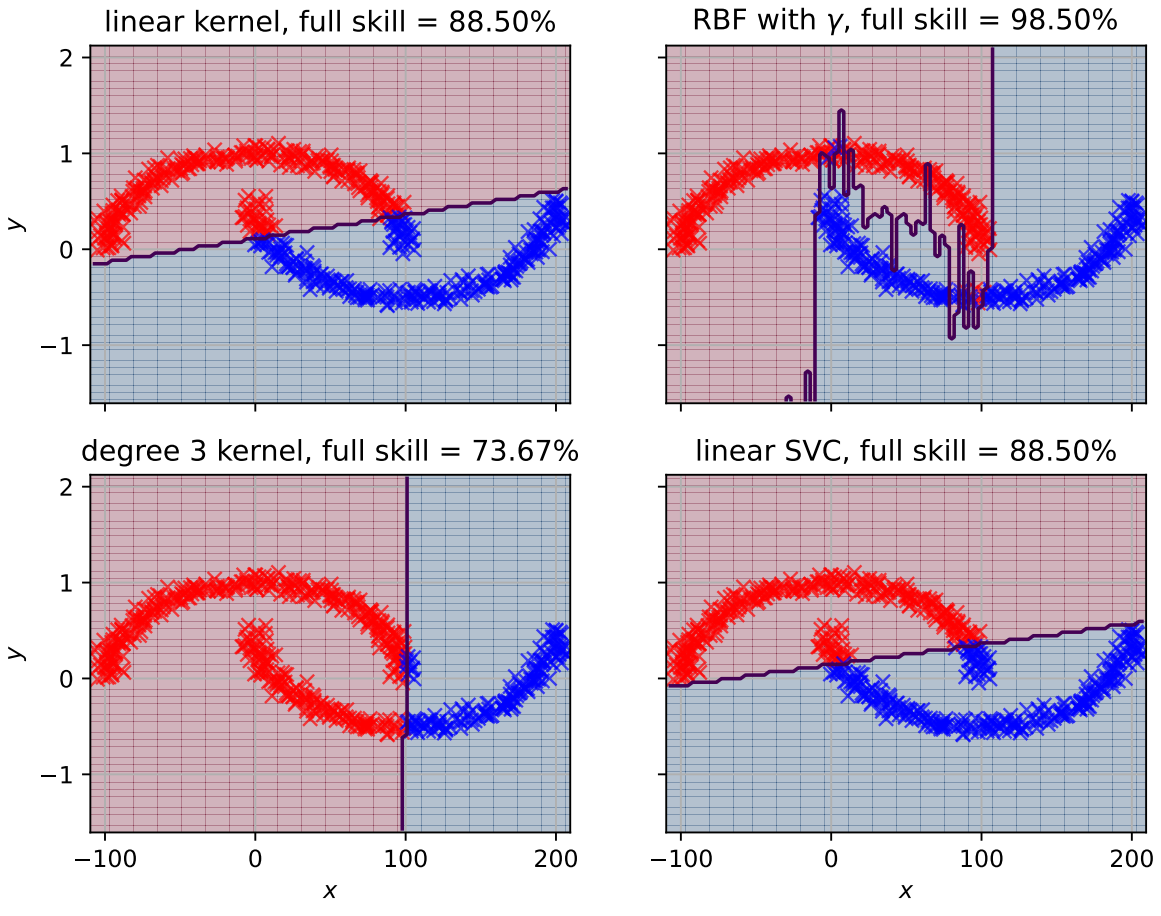

Figure: SVM on stretched moon data with different choices of kernels and regularisations.

Issues with SVM: unbalanced data

- SVM has dependence on sample size, biased towards the larger class

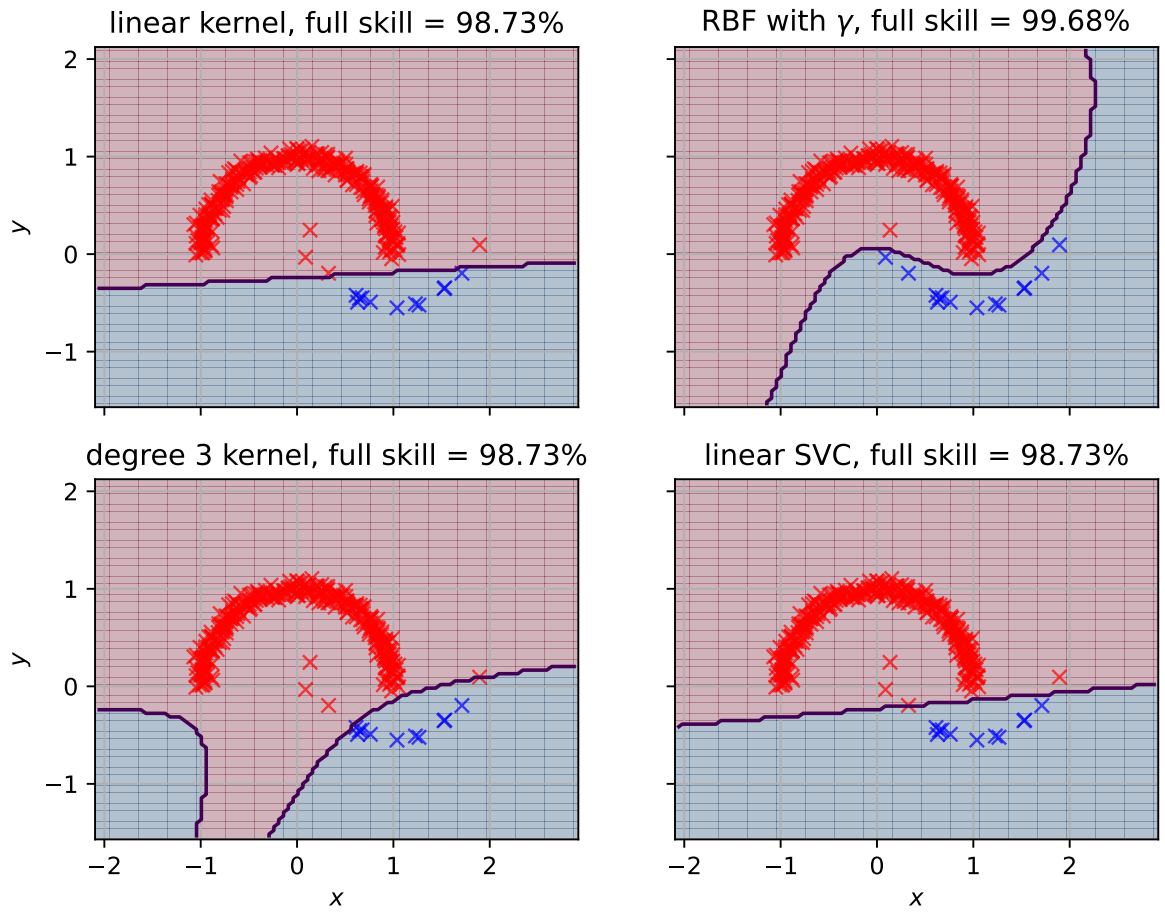

Figure: SVM on unbalanced moon data with different choices of kernels and regularisations.

Issues with SVM: unbalanced data with re-weighting

- one way is to change the weighting on the data

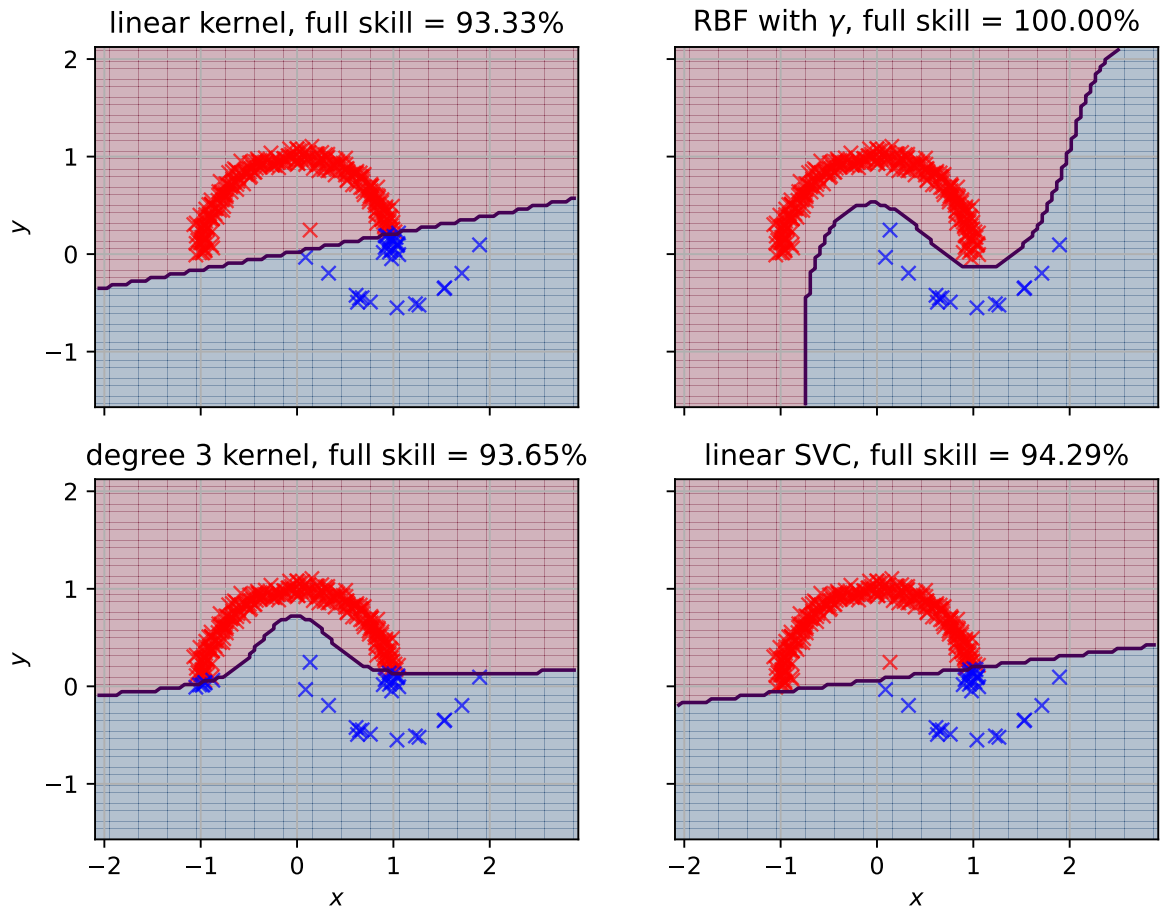

Figure: SVM on unbalanced moon data but with weight rebalancing, with different choices of kernels and regularisations.

Digression: Stochastic Gradient Descent (SGD)

(Relates later to Neural Networks)

- recall loss function J as function of model parameters θ traces out some "landscape" (a hyper-surface), and we want to find the global minimum

  $\rightarrow$ local minimums can exist

Digression: Stochastic Gradient Descent (SGD)

(Relates later to Neural Networks)

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- gradient descent

  $\rightarrow$ compute **full** gradient, find fastest descent

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- gradient descent

  $\rightarrow$ compute **full** gradient, find fastest descent

  $\rightarrow$ can be costly, can get stuck in local minimum

- **stochastic** gradient descent

  $\rightarrow$ **approximates** full gradient by evaluating by computing gradient in only one or a few directions

  $\rightarrow$ take longer to converge, potentially cheaper, could get 'kicked' out of local minimum (that may be a good thing)

Classification as an optimisation problem

- want one-sided loss functions to punish wrong classifications

  $\rightarrow$ samples below; see notebook for description

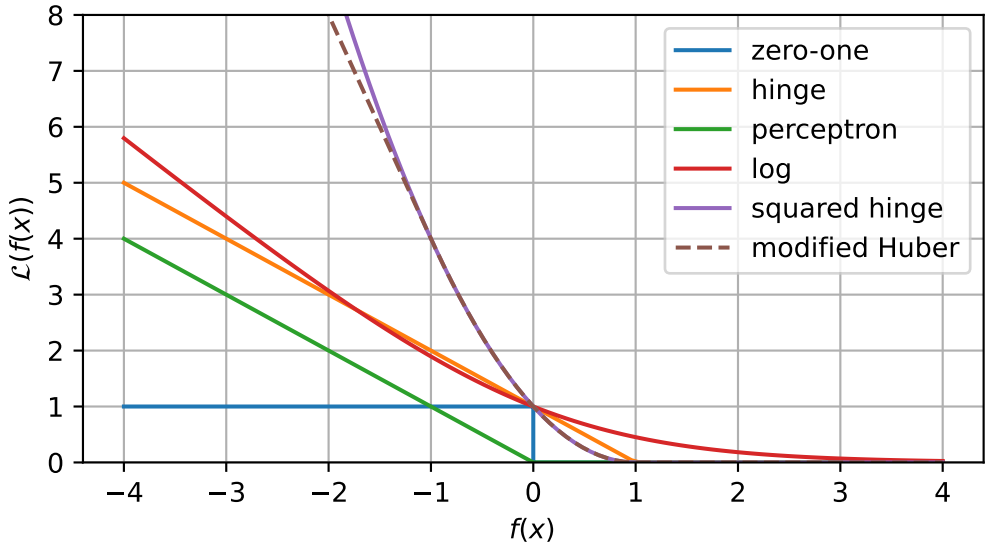


Figure: Selection of loss functions for classification.

- probably want a penalisation too (e.g. L^2, L^1, elastic net)

Special cases

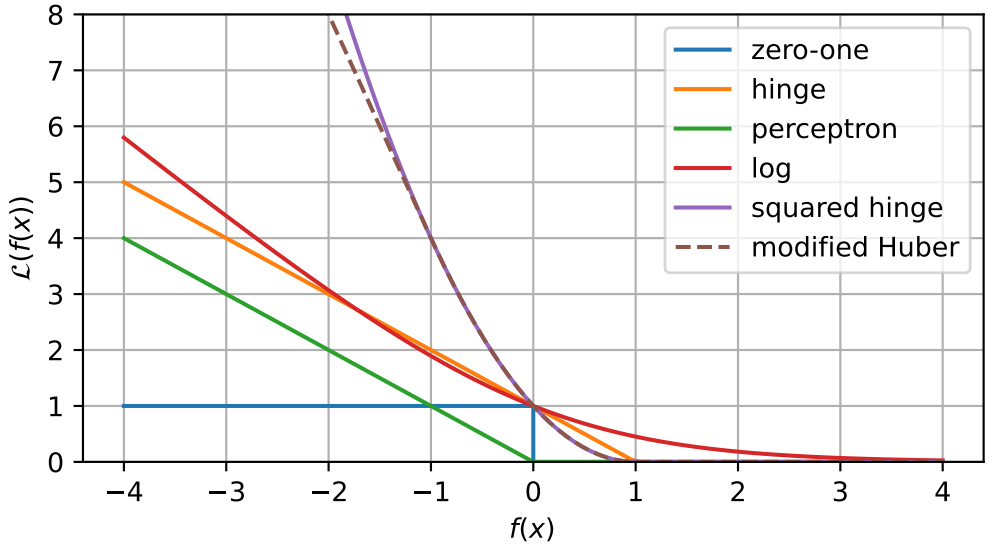


Figure: Selection of loss functions for classification.

- hinge loss + L^2 penalisation $\Rightarrow$ linear SVM
- log loss $\Rightarrow$ logistic regression (a.k.a. logit model, or Maximum Entropy model (not going to elaborate on why)
  $\rightarrow$ it's called 'regression' but it's really classification

- Note: flipping some of these around gives candidates for activation functions (an important component of Networks)

Logistic Regression

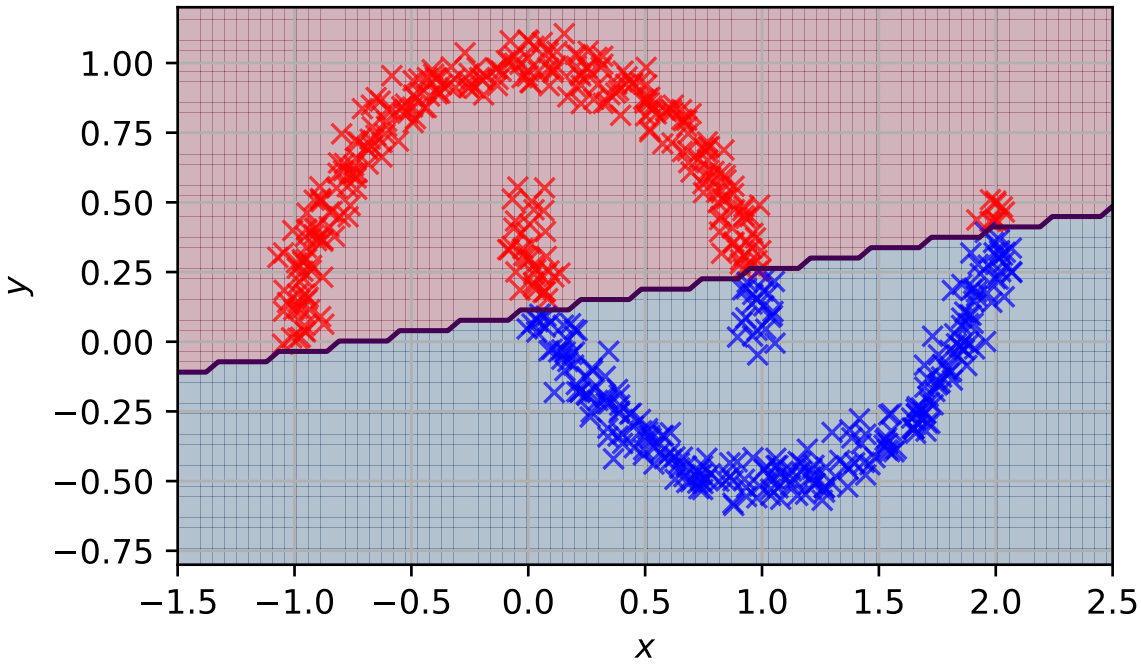


Figure: Logistic regression on moon data with default settings.

- above one is done with `SGDClassifier`

  → more options through `LogisticRegression`

Demonstration: penguins data

- SVM (with rbf) kernel on penguins data

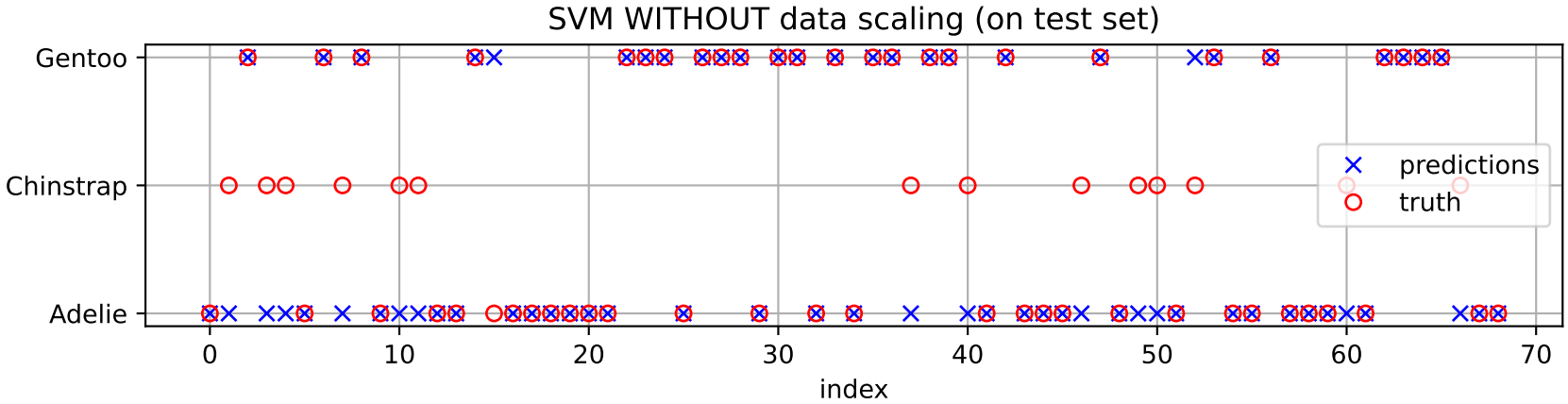
  $\rightarrow$ convert `species` labels to numerical values

  $\rightarrow$ do this wrong first by not scaling the data, using two features (chose the worse combo deliberately)

  $\rightarrow$ scale data, still using two features

  $\rightarrow$ scale data, using all four features

Demonstration: penguins data



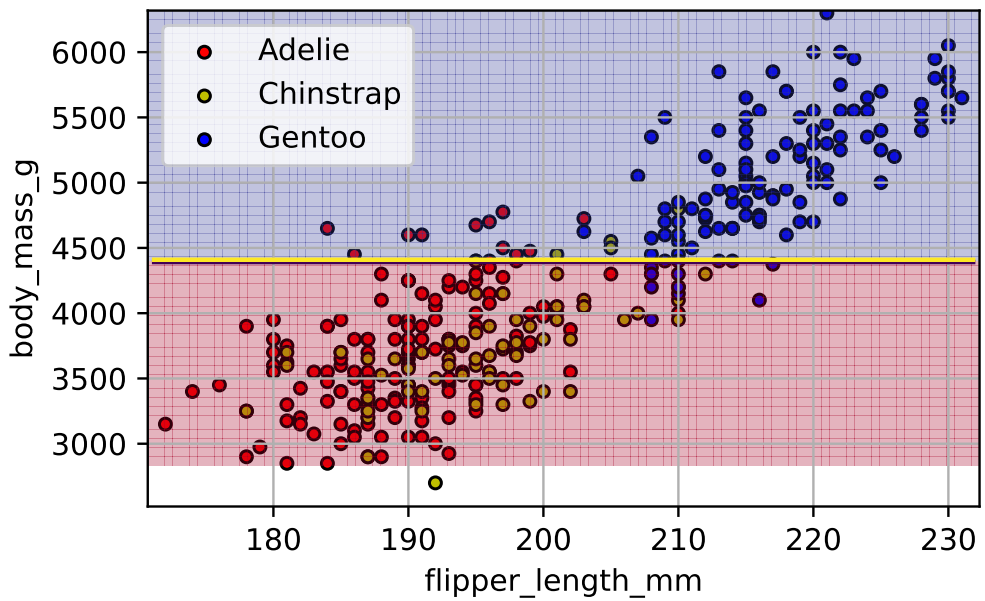


Figure: SVM (with rbf kernel) on **unscaled** penguins data using two features.

Demonstration: penguins data

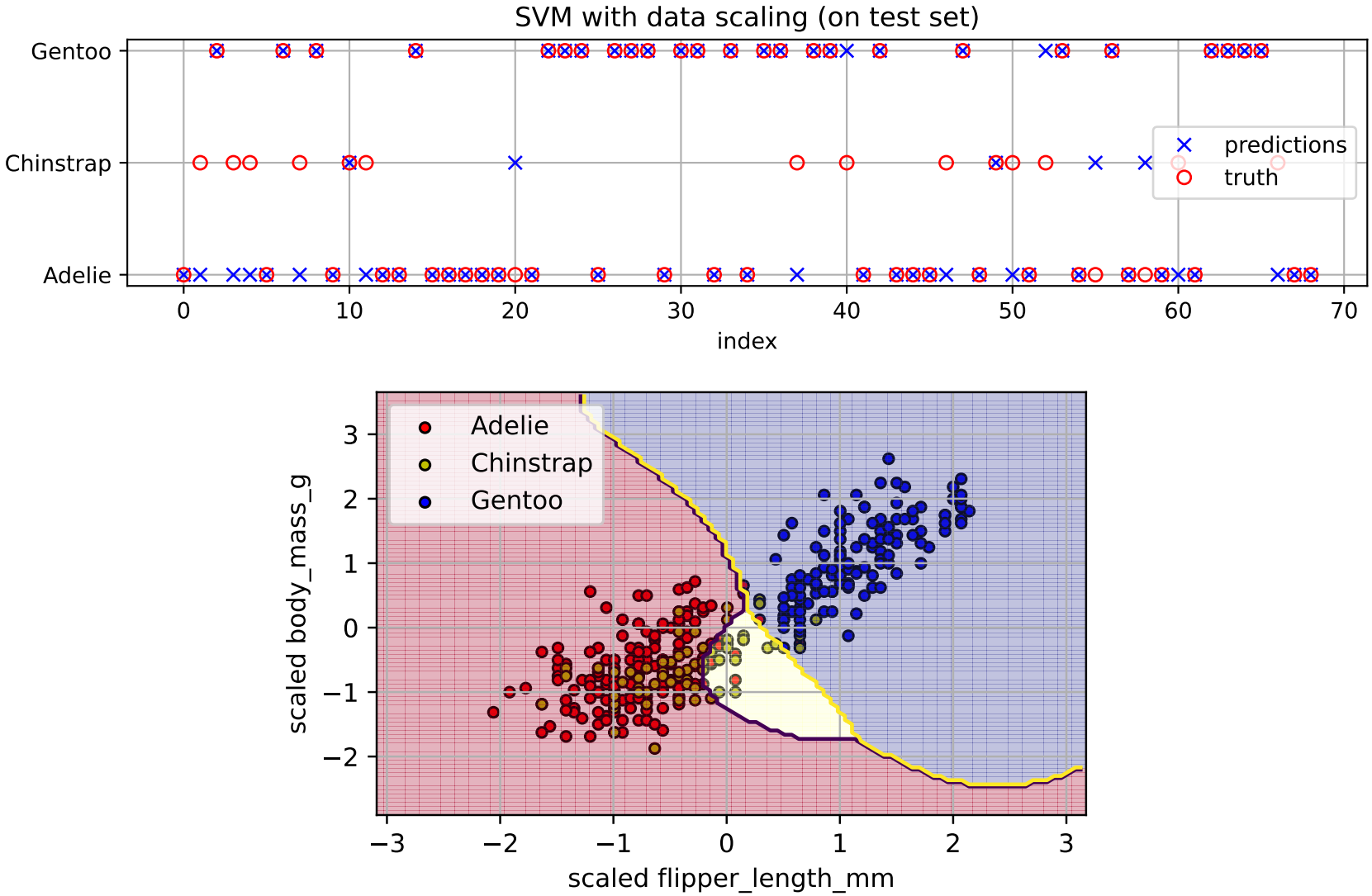


Figure: SVM (with rbf kernel) on scaled penguins data using two features.

Demonstration: penguins data

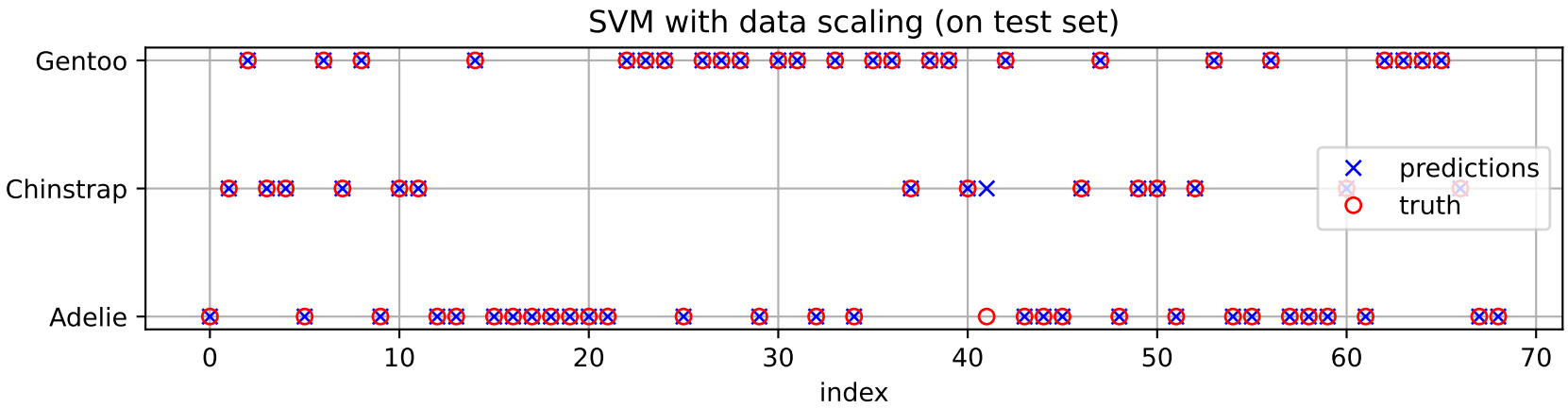


Figure: SVM (with rbf kernel) on scaled penguins data using all features.

- can't show decision boundary here in an obvious way because it lives in 4d

Demonstration

- classification tasks as finding a separator between data

  $\rightarrow$ label prediction
- need to cross-validate and tune hyper-parameters accordingly!

- hard exercise: do image classification

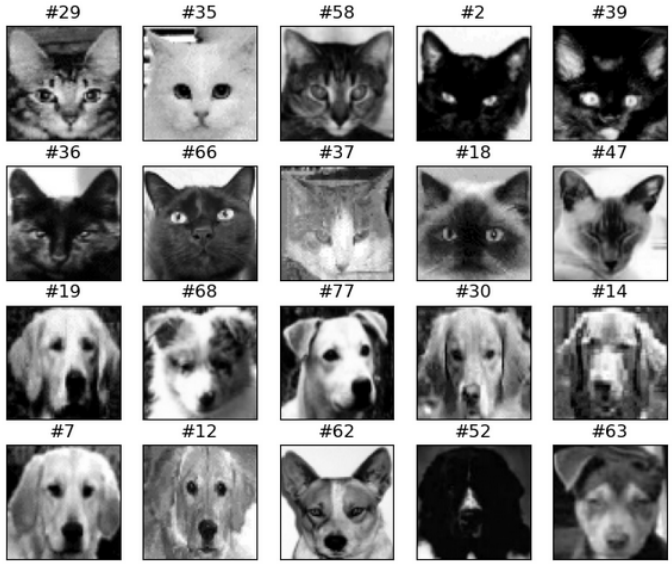


Figure: Selection of cats and dogs as a hard classification task.

Moving to a Jupyter notebook $\rightarrow$