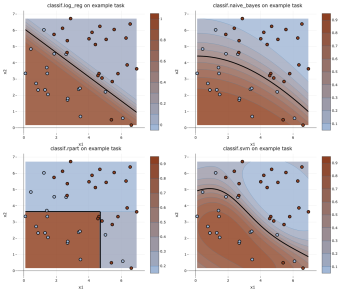
Introduction to Machine Learning

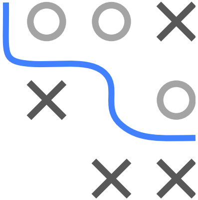
Classification
Basic Definitions



Learning goals

- Basic notation
- Hard labels vs. probabilities vs. scores
- Decision regions and boundaries
- Generative vs. discriminant approaches

NOTATION AND TARGET ENCODING

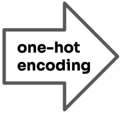


- In classification, we aim at predicting a discrete output

$$y \in \mathcal{Y} = \{C_1, ..., C_g\}$$

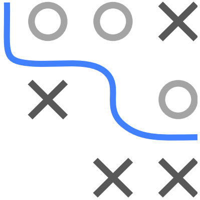
  with $2 \leq g < \infty$, given data $\mathcal{D}$
- For convenience, we often encode these classes differently
- **Binary case,** $g = 2$: Usually use $\mathcal{Y} = \{0, 1\}$ or $\mathcal{Y} = \{-1, +1\}$
- **Multiclass case,** $g \geq 3$: Could use $\mathcal{Y} = \{1, \dots, g\}$, but often use **one-hot encoding** $o(y)$, i.e., g-length vector with $o_k(y) = \mathbb{I}(y = k) \in \{0, 1\}$:

ID	Features	Species
1	...	Setosa
2	...	Setosa
3	...	Versicolor
4	...	Virginica
5	...	Setosa



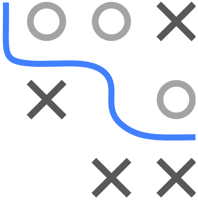
o(Species)
(1, 0, 0)
(1, 0, 0)
(0, 1, 0)
(0, 0, 1)
(1, 0, 0)

CLASSIFICATION MODELS



- While for regression the model $f : \mathcal{X} \to \mathbb{R}$ simply maps to the label space $\mathcal{Y} = \mathbb{R}$, classification is slightly more complicated.
- We sometimes like our models to output (hard) classes, sometimes probabilities, sometimes class scores. The latter 2 are vectors.
- The most basic / common form is the score-based classifier, this is why we defined models already as $f : \mathcal{X} \to \mathbb{R}^g$.
- To minimize confusion, we distinguish between all 3 in notation: $h(\mathbf{x})$ for hard labels, $\pi(\mathbf{x})$ for probabilities and $f(\mathbf{x})$ for scores
- Why all of that and not only hard labels? a) Scores / probabilities are more informative than hard class predictions; b) from an optimization perspective, it is much (!) easier to work with continuous values.

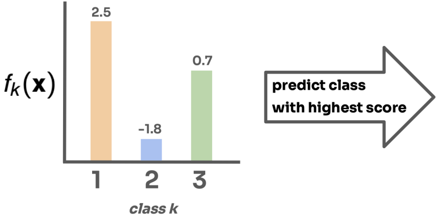
SCORING CLASSIFIERS



- Construct g **discriminant** / **scoring functions** $f_1, ..., f_g : \mathcal{X} \to \mathbb{R}$
- Predicted class is usually the one with max score

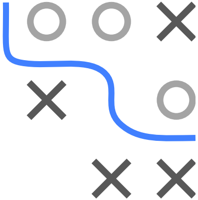
$$h(\mathbf{x}) = \underset{k \in \{1,...,g\}}{\arg\max} \, f_k(\mathbf{x})$$

- For $g = 2$, a single discriminant function $f(\mathbf{x}) = f_1(\mathbf{x}) - f_{-1}(\mathbf{x})$ is sufficient (here, it's natural to label classes with $\{-1, +1\}$ and we used slight abuse of notation for the subscripts), class labels are constructed by $h(\mathbf{x}) = \text{sgn}(f(\mathbf{x}))$
- $|f(\mathbf{x})|$ or $|f_k(\mathbf{x})|$ is loosely called "confidence"



$$h(\mathbf{x}) = \underset{k \in \{1,...,g\}}{\arg\max} \, f_k(\mathbf{x}) = 1$$

PROBABILISTIC CLASSIFIERS



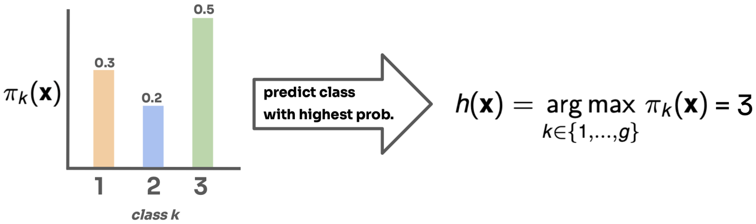
- Construct g **probability functions**

$$\pi_1, \ldots, \pi_g : \mathcal{X} \to [0, 1], \; \sum_{k=1}^{g} \pi_k(\mathbf{x}) = 1$$

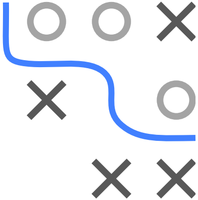
- Predicted class is usually the one with max probability

$$h(\mathbf{x}) = \arg\max_{k \in \{1, \ldots, g\}} \pi_k(\mathbf{x})$$

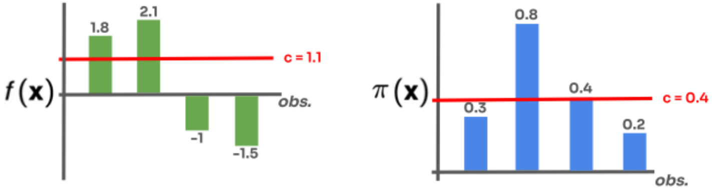
- For $g = 2$, single $\pi(\mathbf{x})$ is constructed, which models the predicted probability for the positive class (natural to encode $\mathcal{Y} = \{0, 1\}$)



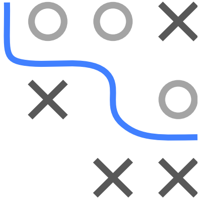
THRESHOLDING



- For imbalanced cases or class with costs, we might want to deviate from the standard conversion of scores to classes
- Introduce basic concept (for binary case) and add details later
- Convert scores or probabilities to class outputs by thresholding: $h(\mathbf{x}) := [\pi(\mathbf{x}) \geq c]$ or $h(\mathbf{x}) := [f(\mathbf{x}) \geq c]$ for some threshold c
- Standard thresholds: $c = 0.5$ for probabilities, $c = 0$ for scores



THRESHOLDING



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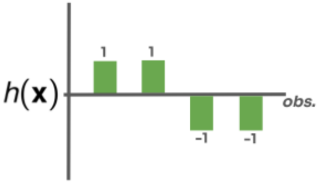
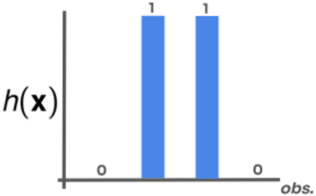
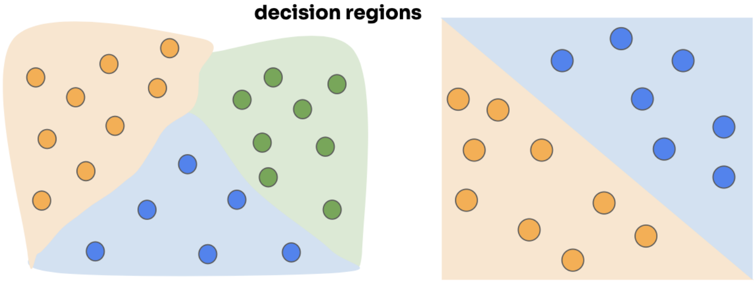


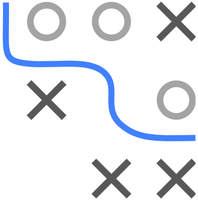


DECISION REGIONS

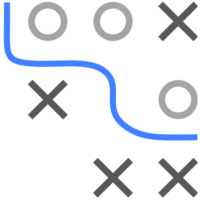
Set of points **x** where class k is predicted:

$$\mathcal{X}_k = \{\mathbf{x} \in \mathcal{X} : h(\mathbf{x}) = k\}$$





DECISION BOUNDARIES



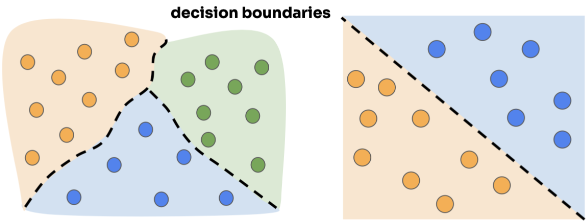
Points in space where classes with maximal score are tied and the corresponding hypersurfaces are called **decision boundaries**

$$\{\mathbf{x} \in \mathcal{X} : \exists\, i \neq j \text{ s.t. } f_i(\mathbf{x}) = f_j(\mathbf{x}) \wedge f_i(\mathbf{x}), f_j(\mathbf{x}) \geq f_k(\mathbf{x})\ \forall k \neq i, j\}$$

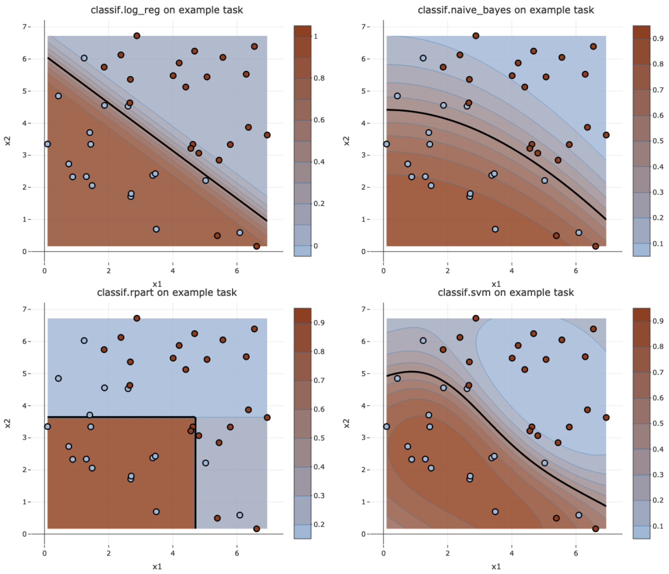
In binary case we can simply use the threshold:

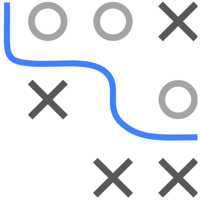
$$\{\mathbf{x} \in \mathcal{X} : f(\mathbf{x}) = c\}$$

$c = 0$ for scores and $c = 0.5$ for probs is consistent with the above.

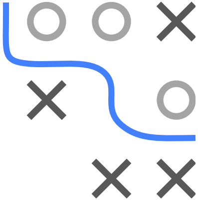


DECISION BOUNDARY EXAMPLES





GENERATIVE APPROACH



Models class-conditional $p(\mathbf{x}|y=k)$, and employs Bayes' theorem:

$$\pi_k(\mathbf{x}) \approx \mathbb{P}(y=k \mid \mathbf{x}) = \frac{\mathbb{P}(\mathbf{x}|y=k)\mathbb{P}(y=k)}{\mathbb{P}(\mathbf{x})} = \frac{p(\mathbf{x}|y=k)\pi_k}{\sum_{j=1}^{g} p(\mathbf{x}|y=j)\pi_j}$$

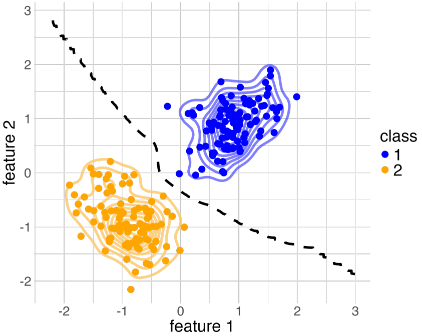
Prior probs $\pi_k = \mathbb{P}(y=k)$ can easily be estimated from training data as relative frequencies of each class:

ID	Sex	Age	Class	Survived the Titanic
1	male	49	2nd	no
2	female	23	1st	yes
3	male	32	3rd	no
4	male	51	2nd	no
5	female	49	1st	yes

$$\hat{\pi} = \frac{2}{5}$$

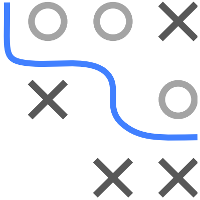
GENERATIVE APPROACH

Decision boundary implicitly defined via the conditional distributions

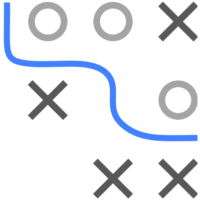


Examples are Naive Bayes, LDA and QDA.

NB: LDA and QDA have ’discriminant’ in their name, but are generative!

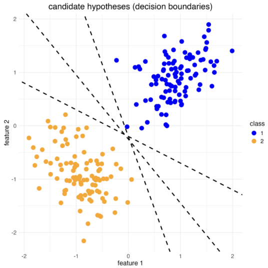


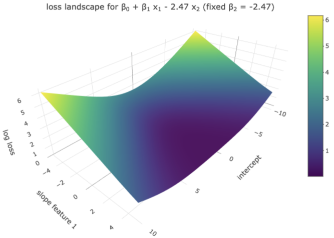
DISCRIMINANT APPROACH

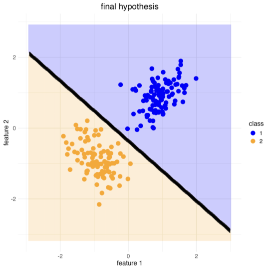


Here we optimize the discriminant functions (or better: their parameters) directly, usually via ERM:

$$\hat{f} = \underset{f \in \mathcal{H}}{\arg\min}\, \mathcal{R}_{\text{emp}}(f) = \underset{f \in \mathcal{H}}{\arg\min} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$







Examples are neural networks, logistic regression and SVMs