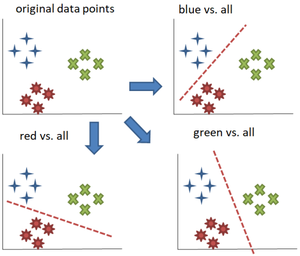
Introduction to Machine Learning

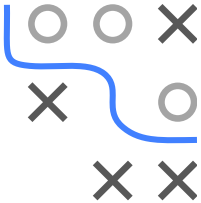
Multiclass Classification
One-vs-Rest and One-vs-One



Learning goals

- Reduce a multiclass problem to multiple binary problems in a model-agnostic way
- Know one-vs-rest reduction
- Know one-vs-one reduction

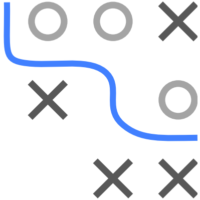
MULTICLASS TO BINARY REDUCTION



- Assume we have a way to train binary classifiers, either outputting class labels $h(\mathbf{x})$, scores $f(\mathbf{x})$ or probabilities $\pi(\mathbf{x})$.
- We are now looking for a model-agnostic reduction principle to reduce a multiclass problem to the problem of solving **multiple binary problems**.
- Two common approaches are **one-vs-rest** and **one-vs-one** reductions.

CODEBOOKS

How binary problems are generated can be defined by a codebook.



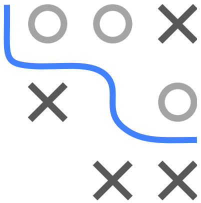
Example:

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	-1
2	-1	1	1
3	0	1	-1

- The k-th column defines how classes of all observations are encoded in the binary subproblem / for binary classifier $f_k(\mathbf{x})$.
- Entry (m, i) takes values $\in \{-1, 0, +1\}$
  - if 0, observations of class $y^{(i)} = m$ are ignored.
  - if 1, observations of class $y^{(i)} = m$ are encoded as 1.
  - if -1, observations of class $y^{(i)} = m$ are encoded as -1.

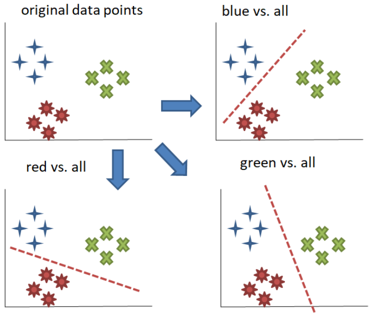
One-vs-Rest

ONE-VS-REST



Create g binary subproblems, where in each the k-th original class is encoded as $+1$, and all other classes (the **rest**) as -1.

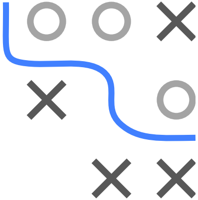
Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	-1
2	-1	1	-1
3	-1	-1	1



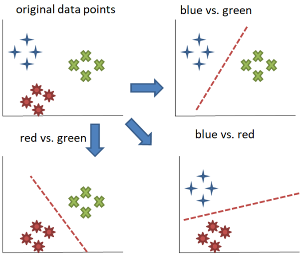
One-vs-One

ONE-VS-ONE

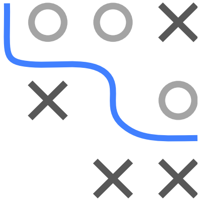
We create $\frac{g(g-1)}{2}$ binary sub-problems, where each $\mathcal{D}_{k,\tilde{k}} \subset \mathcal{D}$ only considers observations from a class-pair $y^{(i)} \in \{k, \tilde{k}\}$, other observations are omitted.



Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	0
2	-1	0	1
3	0	1	-1



COMPARISON ONE-VS-ONE AND ONE-VS-REST



- Note that each binary problem has now much less than n observations!
- For classifiers that scale (at least) quadratically with the number of observations, this means that one-vs-one usually does not create quadratic extra effort in g, but often only approximately linear extra effort in g.
- We experimentally investigate the train times of the one-vs-rest and one-vs-one approaches for an increasing number of classes g.
- We train a support vector machine classifier (SVMs will be covered later in the lecture) on an artificial dataset with $n = 1000$.