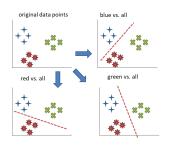
# Introduction to Machine Learning

### 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

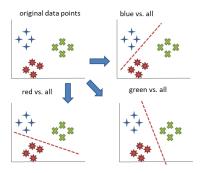
- The k-th column defines how classes of all observations are encoded in the binary subproblem / for binary classifier  $f_k(\mathbf{x})$ .
- Entry (m, l) takes values  $\in \{-1, 0, +1\}$ 
  - if 0, observations of class  $y^{(i)} = m$  are ignored.
  - if 1, observations of class  $y^{(i)} = m$  are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

• Making decisions means applying all classifiers to a sample  $\mathbf{x} \in \mathcal{X}$  and predicting the label k for which the corresponding classifier reports the highest confidence:

$$\hat{y} = \operatorname{arg\ max}_{k \in \{1,2,\ldots,g\}} \hat{f}_k(\mathbf{x}).$$

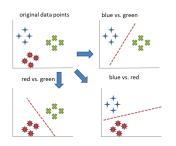
• Obtaining calibrated posterior probabilities is not completely trivial, we could fit a second-stage, multinomial logistic regression model on our output scores, so with inputs  $(\hat{f}_1(\mathbf{x}^{(i)}),...,\hat{f}_g(\mathbf{x}^{(i)}))$  and outputs  $y^{(i)}$  as training data.

## 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



#### **ONE-VS-ONE**

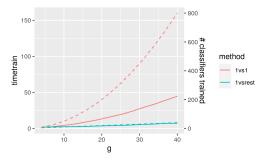
- Label prediction is done via majority voting. We predict the label of a new x with all classifiers and select the class that occurred most often.
- Pairwise coupling (see Hastie, T. and Tibshirani, R. (1998).
  Classification by Pairwise Coupling) is a heuristic to transform scores obtained by a one-vs-one reduction to probabilities.

#### 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.

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

We see that the computational effort for one-vs-one is much higher than for one-vs-rest, but it does not scale proportionally to the (quadratic) number of trained classifiers.



**Figure:** The number of classes vs. the training time (solid lines, left axis) and number of learners (dashed lines, right axis) for each of the two approaches.