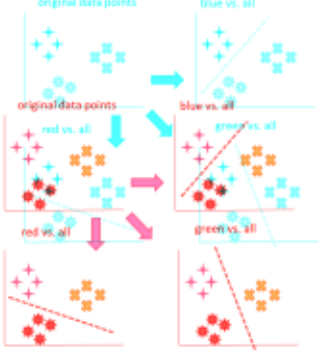
# Introduction to Machine Learning

## 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
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# CODEBOOKS

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

**Example:**

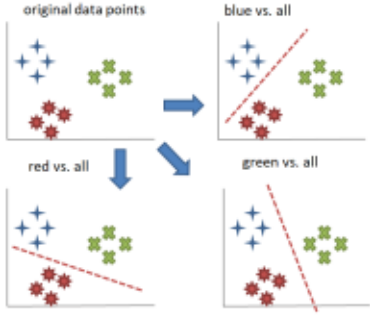
| Class | $f_1(\mathbf{x})$ | $f_2(\mathbf{x})$ | $f_3(\mathbf{x})$ |
|---|---|---|---|
| 1 | 1 | -1 | -1 |
| 2 | -1 | 1 | 1 |
| 3 | 0 | 1 | -1 |

- 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

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 / 2

- 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:

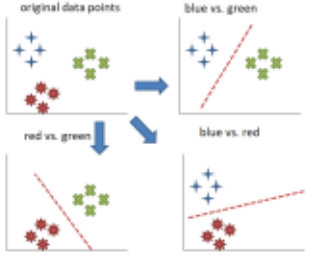
$$\hat{y} = \arg\max_{k \in \{1,2,\ldots,g\}} \hat{f}_k(\mathbf{x}).$$

- 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 $\left(\hat{f}_1(\mathbf{x}^{(i)}), \ldots, \hat{f}_g(\mathbf{x}^{(i)})\right)$ and outputs $y^{(i)}$ as training data.

# 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 / 2

- 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 / 2

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.

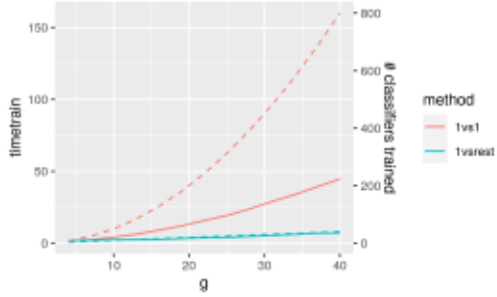



**Figure:** The number of classes vs. the training time (solid lines, left axis) and number of learners (dashed lines, right axis) for each of the two approaches.