Reduction to Binary Classification

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Slides based on Lecture 09 from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

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Overview

Motivation

- So far, most algorithms we've learned are designed for binary classification.
- Many real-world problems have more than two classes.
- [discussion]What are some potential issues when we have a large number of classes?

Today's lecture

- How to *reduce* multiclass classification to binary classification?
- How do we *generalize* binary classification algorithm to the multiclass setting?
- Example of very large output space: structured prediction.

Reduction to Binary Classification

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train k binary classifiers, one for each class: $h_1, \ldots, h_k : \mathcal{X} \to \mathbf{R}$.
- Classifier h_i distinguishes class i (+1) from the rest (-1).

Prediction

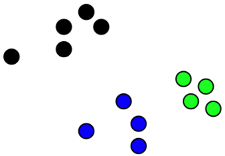
- Majority vote:

$$h(x) = \underset{i \in \{1, \ldots, k\}}{\arg\max}\, h_i(x)$$

- Ties can be broken arbitrarily.

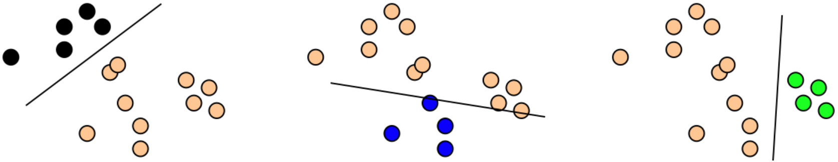
OvA: 3-class example

Consider a dataset with three classes:



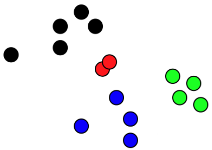
Assumption: each class is linearly separable from the rest.
Ideal case: only target class has positive score.

Train OvA classifiers:



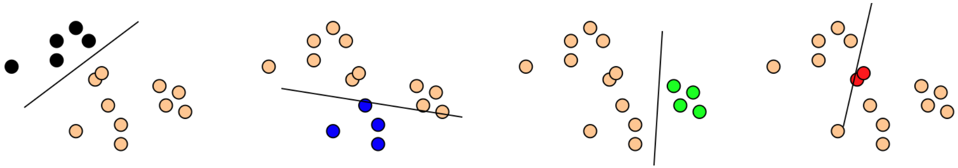
OvA: 4-class non-separable example

Consider a dataset with four classes:



Cannot separate red points from the rest.
Which classes might have low accuracy?

Train OvA classifiers:



All vs All / One vs One / All pairs

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathbf{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
- Classifier h_{ij} distinguishes class i (+1) from class j (-1).

Prediction

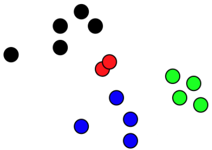
- Majority vote (each class gets $k-1$ votes)

$$h(x) = \underset{i \in \{1,\ldots,k\}}{\arg\max} \sum_{j \neq i} \underbrace{h_{ij}(x)\mathbb{I}\{i < j\}}_{\text{class } i \text{ is } +1} - \underbrace{h_{ji}(x)\mathbb{I}\{j < i\}}_{\text{class } i \text{ is -1}}$$

- Tournament
- Ties can be broken arbitrarily.

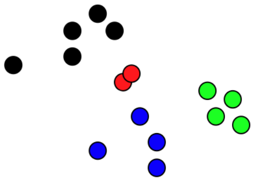
AvA: four-class example

Consider a dataset with four classes:



Assumption: each pair of classes are linearly separable.
More expressive than OvA.

What's the decision region for the red class?



[discussion]OvA vs AvA

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$
challenges	train	class imbalance	small training set
	test	calibration / scale tie breaking	

Lack theoretical justification but simple to implement and works well in practice (when # classes is small).

Question: When would you prefer AvA / OvA?

Code word for labels

Using the reduction approach, can you train fewer than k binary classifiers?

Key idea: Encode labels as binary codes and predict the code bits directly.

OvA encoding:

class	h_1	h_2	h_3	h_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1

OvA uses k bits to encode each label, what's the minimal number of bits you can use?

Error correcting output codes (ECOC)

Example: 8 classes, 6-bit code

class	h_1	h_2	h_3	h_4	h_5	h_6
1	0	0	0	1	0	0
2	1	0	0	0	0	0
3	0	1	1	0	1	0
4	1	1	0	0	0	0
5	1	1	0	0	1	0
6	0	0	1	1	0	1
7	0	0	1	0	0	0
8	0	1	0	1	0	0

Training Binary classifier h_i:

- +1: classes whose i-th bit is 1
- -1: classes whose i-th bit is 0

Prediction Closest label in terms of Hamming distance.

h_1	h_2	h_3	h_4	h_5	h_6
0	1	1	0	1	1

Code design Want good binary classifiers.

Error correcting output codes: summary

- Computationally more efficient than OvA (a special case of ECOC). Better for large k.
- Why not use the minimal number of bits ($\log_2 k$)?
  - If the minimum Hamming distance between any pair of code word is d, then it can correct $\left\lfloor \frac{d-1}{2} \right\rfloor$ errors.
  - In plain words, if rows are far from each other, ECOC is robust to errors.
- Trade-off between code distance and binary classification performance.
- Nice theoretical results [Allwein et al., 2000] (also incoporates AvA).

Review

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA, ECOC.
- Key is to design "natural" binary classification problems without large computation cost.

But,

- Unclear how to generalize to extremely large # of classes.
- ImageNet: >20k labels; Wikipedia: >1M categories.

Next, generalize previous algorithms to multiclass settings.