Reductions

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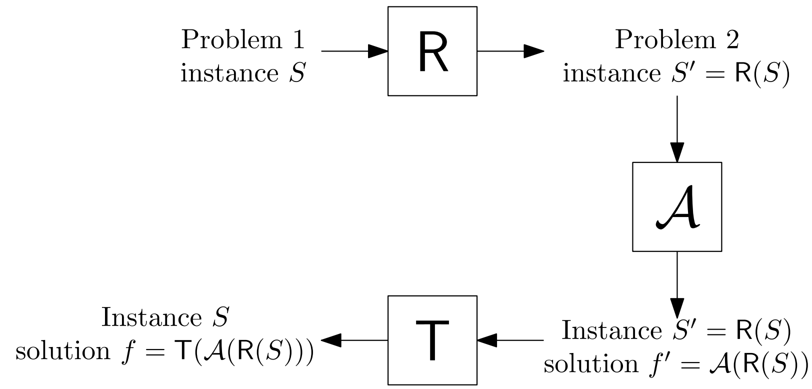

In machine learning, typically have

- Problem 1: the problem you have to solve for a real application
- Problem 2: a well-studied problem in machine learning
- Problem instance: training data and (implicitly) a probability distribution P
- Solution: prediction functions
- $\mathcal{A}$: the latest, greatest learning algorithm for Problem 2

Examples

0. **Problem**: binary classification
   - **Reduction**: boosting
     (Reduces problem to binary classification.)
1. **Problem**: importance-weighted classifiation
   - **Reduction**: rejection sampling
     (Reduces problem to unweighted classification.)
2. **Problem**: multi-class classification
   - **Reduction**: One-Against-All
     (Reduces problem to binary classification.)

Importance-weighted classification

Problem:

- **Setting**: Random triple $(X, Y, C) \sim P$ for some probability distribution P over $\mathcal{X} \times \mathcal{Y} \times \mathbb{R}_+$.
  $C =$ **importance weight** for labeled example (X, Y).
- **Goal**: Function $f \colon \mathcal{X} \to \mathcal{Y}$ with small **importance-weighted error**:

$$\mathbb{E}\Big[C \cdot \mathbb{1}\{f(X) \neq Y\}\Big].$$

Problem instance:

- Training data S: collection of triples $(x, y, c) \in \mathcal{X} \times \mathcal{Y} \times \mathbb{R}_+$, presumed to be drawn i.i.d. from P.

Where it comes up:

- *Class-specific weights*: e.g., $C = 100 \Leftrightarrow Y = 0$ (and $C = 1$ otherwise).
- *Input-specific weights*: e.g., $C = 100 \Leftrightarrow X \in \mathcal{X}_0$ (and $C = 1$ o.w.).
- *Boosting*, *domain adaptation*, *causal inference*, ...

(Note: many learning algorithms natively handle importance weights.)

Would like to reduce to (unweighted) classification.

The rejection sampling reduction

Main idea: Transform training data S so it looks like it came from a distribution P', where

$$\mathbb{E}_{(X,Y,C)\sim P}\Big[C \cdot \mathbb{1}\{f(X) \neq Y\}\Big] = \mathbb{E}_{(X',Y')\sim P'}\Big[\mathbb{1}\{f(X') \neq Y'\}\Big].$$

Instance mapping procedure

Input Training data S from $\mathcal{X} \times \mathcal{Y} \times \mathbb{R}_+$.

1: Initialize $S' = \emptyset$.
2: Let $c_{\max} := \max_{(x,y,c)\in S} c$.
3: **for** each $(x, y, c) \in S$ **do**
4: Toss a coin with $\Pr(\text{heads}) = \frac{c}{c_{\max}}$.
5: If heads, keep example—put (x, y) into S'.
6: If tails, discard example.
7: **end for**
8: **return** Training data S' from $\mathcal{X} \times \mathcal{Y}$.

Solution mapping procedure: identity map

The rejection sampling reduction

Why rejection sampling works: (Assume for simplicity that $c_{\max} = 1$.)

Define random variable

$$Q := \mathbb{1}\{\text{Keep example } (X, Y)\}$$

which, after conditioning on (X, Y, C), has mean C.

Distribution of examples in S' is same as that of (X, Y) conditioned on $Q = 1$.

Moreover,

$$\begin{aligned}\mathbb{E}\Big[Q \cdot \mathbb{1}\{f(X) \neq Y\}\Big] &= \mathbb{E}\Big[\mathbb{E}\Big[Q \cdot \mathbb{1}\{f(X) \neq Y\} \,\Big|\, (X, Y, C)\Big]\Big] \\ &= \mathbb{E}\Big[C \cdot \mathbb{1}\{f(X) \neq Y\}\Big]\end{aligned}$$

Conclusion:
Error rate w.r.t. P' $\propto$ importance-weighted error rate w.r.t. P.

Multi-class classification

Problem:

- **Setting**: Random pair $(X, Y) \sim P$ for some probability distribution P over $\mathcal{X} \times \{1, 2, \ldots, K\}$.
- **Goal**: Function $f : \mathcal{X} \to \mathcal{Y}$ with small prediction error $P(f(X) \neq Y)$.

Problem instance:

- Training data S: collection of pairs $(x, y) \in \mathcal{X} \times \{1, 2, \ldots, K\}$, presumed to be drawn i.i.d. from P.

Would like to reduce to binary classification.

One-Against-All reduction

Main idea: Create K binary classification problems

given $x \in \mathcal{X}$, predict whether or not $y = i$.

Create K examples from each $(x, y) \in S$:

$$(x, y) \longrightarrow \begin{cases} (x, \mathbb{1}\{y = 1\}) & \longrightarrow & S'_1 \\ (x, \mathbb{1}\{y = 2\}) & \longrightarrow & S'_2 \\ \vdots & \vdots & \vdots \\ (x, \mathbb{1}\{y = K\}) & \longrightarrow & S'_K \end{cases}$$

One-Against-All reduction

Instance mapping procedure

Input Training data S from $\mathcal{X} \times \{1, 2, \ldots, K\}$.

1: Initialize empty sets $S'_1, S'_2, \ldots, S'_K$.
2: **for** each $(x, y) \in S$ **do**
3: **for** each $i = 1, 2, \ldots, K$ **do**
4: Put $(x, \mathbb{1}\{y = i\}) \in \mathcal{X} \times \{0, 1\}$ into S'_i.
5: **end for**
6: **end for**
7: **return** Training data sets $S'_1, S'_2, \ldots, S'_K$ from $\mathcal{X} \times \{0, 1\}$.

Solution mapping procedure

Input K binary predictors $f'_1, f'_2, \ldots, f'_K : \mathcal{X} \to \{0, 1\}$.

return Function $f : \mathcal{X} \to \{1, 2, \ldots, K\}$ where

$$f(x) = \underset{i \in \{1,2,\ldots,K\}}{\arg\max} \; f'_i(x) \quad \text{(breaking ties arbitrarily).}$$

This should seem werid!

Problem with OAA

OAA multi-class predictor:

$$f(x) \;=\; \underset{i \in \{1,2,\ldots,K\}}{\arg\max} \; f'_i(x) \,.$$

Only get correct classification on (x, y) if $f'_y(x) = 1$ and $f'_i(x) = 0$ for all $i \neq y$.
(Could err if any of the f'_i errs!)

Solution: use conditional probability estimation

$$f'_i(x) \;=\; \text{estimate of } P(Y = i \mid X = x) \,.$$

Comparing OAA and ECOC

Empirical comparison

Many reductions for multi-class—not all work equally well!

- Eight multi-class problems (from the UCI repository).
- $\mathcal{A}$ = `classregtree` from the MATLAB statistics toolbox, estimate conditional probabilities using square loss.
- Compare One-against-all (OAA) to Error Correcting Output Codes (ECOC).

Data set	Number of classes	OAA	ECOC
ecoli	8	0.0985	**0.0517**
glass	6	0.3874	**0.3462**
pendigits	10	0.0985	**0.0517**
satimage	6	0.1679	**0.1376**
soybean	19	0.6580	**0.5993**
splice	3	**0.0642**	0.0699
vowel	11	0.6356	**0.5780**
yeast	10	0.4893	**0.4479**

Summary

- **Reductions**: reuse existing technology to solve new problems.
  - Multi-class (OAA, ECOC, tournaments, . . .)
  - Multi-label prediction
  - Ranking
  - Sequence prediction
  - . . .
- **Lots of different problems and objectives** beyond binary classificaiton and prediction error—can be application-/domain-specific.

Key takeaways

1. Concept of reductions.
2. Reduction for importance-weighted classification.
3. OAA reduction for multi-class.
4. Importance of conditional probability estimation.