Practical tricks

Machine Learning and Data Mining

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Outline

Here, we consider practical problems that are not quite aligned with theory:

- imbalanced datasets;
- differences in training and application domains;
- one-class classification.

Imbalanced datasets

Imbalanced datasets

Settings:

- classification problem: $\mathcal{C}^+$ against $\mathcal{C}^-$;
- often in practice $P(\mathcal{C}^+) \ll P(\mathcal{C}^-)$.

This poses several problems:

- mini-batch learning procedures degradate;
  - extreamely slow learning;
- imprecise results.

Degradation of mini-batch learning

Probability of a example from $\mathcal{C}^+$ being selected into a mini-batch is low:

- $\Rightarrow$ increased $\mathbb{D}[\nabla\mathcal{L}]$;
- $\Rightarrow$ low learning rate;
- $\Rightarrow$ slow learning.

Changing priors

$$P(\mathcal{C}^+ \mid X) \quad = \quad \frac{P(X \mid \mathcal{C}^-)P(\mathcal{C}^-)}{P(X \mid \mathcal{C}^-)P(\mathcal{C}^-) + P(X \mid \mathcal{C}^+)P(\mathcal{C}^+)};$$

$$\frac{L^+}{L^-} \quad = \quad \frac{P(\mathcal{C}^+ \mid X)}{P(\mathcal{C}^- \mid X)} = \frac{P(X \mid \mathcal{C}^+)}{P(X \mid \mathcal{C}^-)} \cdot \frac{P(\mathcal{C}^+)}{P(\mathcal{C}^-)}.$$

Let $\mathcal{D}[h] = \{\{x \mid h(x) > \tau\} \mid \tau \in \mathbb{R}\}$ i.e. set of decision surfaces.

$f(x) = P(\mathcal{C}^+ \mid X)$ - the ideal classifier for $\mathcal{C}^+$ against $\mathcal{C}^-$.

$$\mathcal{D}[f] = \mathcal{D}\left[\frac{f}{1-f}\right] = \mathcal{D}\left[\frac{L^+}{L^-}\right] = \mathcal{D}\left[\frac{P(X \mid \mathcal{C}^+)}{P(X \mid \mathcal{C}^-)}\right]$$

Changing priors

An ideal classifier:

- invariant to change of priors w.r.t. set of decision surfaces;
- change of priors might stabilize and speed up learning;
- **only true for a really good classifiers!**

Not ideal classifier under change of priors:

- low capacity classifiers might change surfaces significantly;
- dramatic changes of priors may render classifier useless.

Sampling

- slow convergence is a result high gradient variance;
- which is the result of unstable composition of mini-batches.

Solutions:

- stratified batches (forcing class ratio into batches);
- change in sampling distribution (importance sampling).

Importance sampling

$$\mathcal{L} = \mathbb{E}_{x,y\sim P_{x,y}} l(f(x), y) =$$

$$\int_{x,y} P(x,y) l(f(x),y) dxdy =$$

$$\int_{x,y} P'(x,y) \frac{P(x,y)}{P'(x,y)} l(f(x),y) dxdx =$$

$$\mathbb{E}_{x,y\sim P'_{x,y}} w(x,y) l(f(x),y).$$

$w(x,y) = \frac{P(x,y)}{P'(x,y)}$ - weights.

Importance sampling

Resampling trick allows to:

- stabilize increase frequency of rare but important samples;
- increase speed of convergence.

Importance can be predetermined e.g.:

- uniform sampling across classes;
- increased sampling probability of hard examples.

Weights can be computed on the fly e.g. adaptive sampling methods.

Reweighting

Reweighting

Settings:

- training set X with distribution P;
- target set X' with distribution P' but with absent targets;
- $P(x) \neq P'(x)$, but
- $\operatorname{supp} P = \operatorname{supp} P'$.

Examples:

- training on results of computer simulations.

Reweighting

- train a classifier $r(x)$ on X' against X:

$$w(x) = \frac{r(x)}{1 - r(x)} = \frac{P'(x)}{P'(x) + P(x)} \cdot \frac{P'(x) + P(x)}{P(x)} = \frac{P'(x)}{P(x)}$$

- use output as weights (similar to importance sampling):

$$\mathcal{L}_{\text{target}} = \mathop{\mathbb{E}}_{x,y \sim P'} l(f(x), y) = \mathop{\mathbb{E}}_{x,y \sim P} w(x) l(f(x), y)$$

BDT reweighting

Boosting training scheme allows for an especially efficient reweighting algorithm:

- $w^0(x) = 1$
- repeat until new classifier yield random guess performance:
  - train new classifier f^t on X' against X with weights $w^t(x)$;
  - $w^{t+1}(x) = w^t(x) \frac{f^t(x)}{1-f^t(x)}$.

Semi-supervised learning

Settings

Semi-supervised learning targets cases with a large amount of unlabeled data:

- $\mathcal{D}_{\text{supervised}} = \{(x_i, y_i)\}_{i=1}^{N}$;
- $\mathcal{D}_{\text{unsupervised}} = \{x_i\}_{i=1}^{M}$;
- $|\mathcal{D}_{\text{unsupervised}}| \gg |\mathcal{D}_{\text{supervised}}|$;
- distributions of X are equal in both datasets.
- also can be used for unbalanced datasets.

Semi-supervised learning

Common techniques:

- train dimensionality reduction method on $\mathcal{D}_{\text{unsupervised}}$;
- apply dimensionality reduction to $\mathcal{D}_{\text{supervised}}$;
- solve supervised problem reduced domain.

Examples:

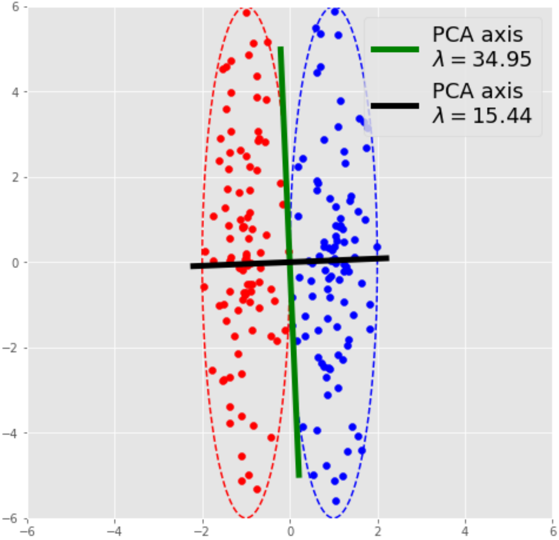
- feature selection + classifier;
- PCA + classifier.

Semi-supervised learning

Dimensionality reduction and supervised methods are trained independently:

- conflict of objectives:
    - reducing dimensionality without losses $\neq$ easier supervised problem;
    - information lost in compression might be important for supervised task.

Conflict of objectives



Semi-supervised deep learning

In Deep Learning both objectives (dimensionality reduction and supervised task) can be trained simultaneously, e.g.:

- encoder $z = e(x)$;
- decoder $x' = d(z)$;
- classifier $f(z)$

$$\mathcal{L} = \mathop{\mathbb{E}}_{X,Y \sim \text{supervised}} l_1(f(e(x)), y) + \lambda \mathop{\mathbb{E}}_{X \sim \text{unsupervised}} l_2(x, d(e(x)))$$

One-class classification

Settings

- training dataset consist only from one class $\mathcal{C}^+$;
- target dataset might contain additional classes.

Examples:

- anomaly detection;
- outlier detection;
- novelty detection.

One-class classification

Density based:

- decision function: $P(X|\mathcal{C}^+) > \tau$;
- essentially, generative problem;

Distance based:

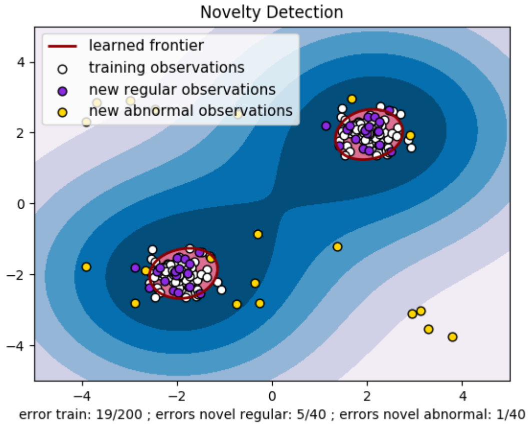
- well, a distance is employed...
- $d(x, ?) < \tau$.

One-class SVM

Minimizes volume contained by class:

$$
\begin{aligned}
\min \frac{1}{2}\|w\|^2 \quad &+ \quad \frac{1}{\nu n}\sum_i \left[\xi_i - \rho\right] \\
\text{subject} \quad & \quad \text{to} \\
w\phi(x_i) \geq \rho - \xi_i \quad &: \quad \forall i \\
\xi_i \geq 0 \quad &: \quad \forall i
\end{aligned}
$$

One-class SVM



Source: sklearn

Dimensionality reduction

The following heuristic might help:

- train an Auto-Encoder e, d on positive class;
- compute distribution of reconstruction errors $P\left[(x - d(e(x)))^2\right]$;
- use this distribution as score for one-class classification:

$$P\left[(x - d(e(x)))^2\right] > \tau$$

- Auto-Encoder should be heavily restricted;
- better to use denoising AE:

$$\sum_i \left[x_i - d(e(x_i + \varepsilon))\right]^2 \to \min$$

Restricted networks

Some use a network:

- $f(x)$ trained to replicate $y(x) = 1$;
- f is heavily restricted:
  - bottleneck does not allow to learn $y(x) = 1$ for all x.

Examples:

- Radial Basis Networks:

$$f(x) = \sum_i w_i \exp(-\|x - c_i\|^2)$$

One against everything

One against everything = semi-supervised + one-class:

- large unlabeled dataset $\mathcal{D}$;
- small positive dataset $\mathcal{C}^+$;
- train positive class against everything:

$$f(x) = \frac{P(X \mid \mathcal{C}^+)}{P(X \mid \mathcal{C}^+) + P(X \mid \mathcal{D})} \sim P(X \mid \mathcal{C}^+)$$

One against everything

Examples:

- it is easy to sample large amounts of text (e.g. tweets);
- sampling abnormal text might be problematic.

Summary

Summary

Imbalanced datasets:

- **be careful with changing priors**;
- resampling.

Importance sampling:

- may improve convergence and stability;
- importance sampling optimization improves convergence rate.

Summary

Reweighting:

- different training and target distributions of X.
- a special case of domain adaptation.

One-class classification:

- a very strange field;
- usually, ill-defined problem.