Practical tricks

Machine Learning and Data Mining

Maxim Borisyak
National Research University Higher School of Economics (HSE)

October 11, 2017

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

$$\mathcal{L} = \mathbb{E}_{x,y\sim P_{x,y}} l(f(x), y) = \int_{x,y} P(x,y) l(f(x), y) dx dy = \int_{x,y} P'(x,y) \frac{P(x,y)}{P'(x,y)} l(f(x), y) dx dx = \mathbb{E}_{x,y\sim P'_{x,y}} w(x,y) l(f(x), y).$$

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

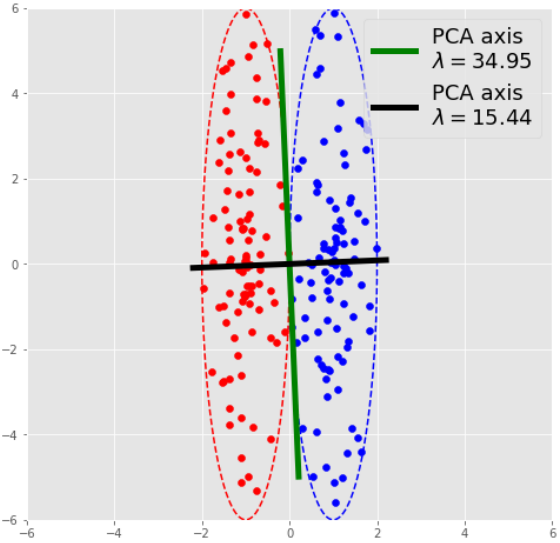
- feature selection + classifier;
- PCA + classifier.

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

Essentially, generative problem:

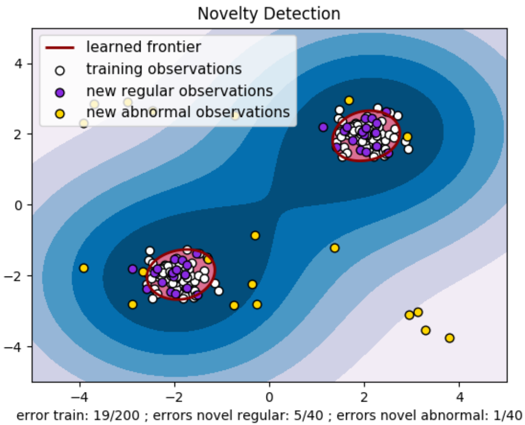
- decision function: $P(X|\mathcal{C}^{+}) > \tau$;
- however, objective is a classification one w.r.t unknown class;
- thus, ill-defined problem.

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.

Reweighting:

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

One-class classification:

- a very strange field;
- ill-defined generative problem.