No Free Lunch

Machine Learning and Data Mining

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No free lunch

IQ test: try to learn yourself!

First question from MENSA website:
Following the pattern shown in the number sequence below, what is the missing number?

$$1, 8, 27, ?, 125, 216$$

Possible answers:

- 36
- 45
- 46
- 64
- 99

IQ test: try to learn yourself!

First question from MENSA website:
Following the pattern shown in the number sequence below, what is the missing number?

X_{train}	1	2	3	5	6
y_{train}	1	8	27	125	216

$$X_{\text{test}} = (4,)$$

IQ test: try to learn yourself!

My solution:

$$y = \frac{1}{12}(91x^5 - 1519x^4 + 9449x^3 - 26705x^2 + 33588x - 14940)$$

- fits perfectly!

My answer:

- 99

IQ test

Why solution:

$$y = x^3$$

seems much more suitable than

$$y = \frac{1}{12}(91x^5 - 1519x^4 + 9449x^3 - 26705x^2 + 33588x - 14940)?$$

Terminology

Machine Learning is about learning algorithms A that:

- defined on sample set $\mathcal{X}$ (e.g. $\mathbb{R}^n$) and targets $\mathcal{Y}$ (e.g. $\{0, 1\}$):
    - $\mathcal{X}$ and $\mathcal{Y}$ are discrete;
- take a problem (dataset) $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$;
- learn relation between $\mathcal{X}$ and $\mathcal{Y}$;
- and return prediction function h (hypothesis):

$$\begin{aligned} A(D) &= h \\ h : \mathcal{X} &\to \mathcal{Y} \end{aligned}$$

By this definition, e.g. XGBoost is a **family** of algorithms.

Off-training-set error

$$\mathrm{Err}(f, h, d) = \frac{\sum_{x \in d_X} \pi(x) \mathbb{I}[f(x) \neq h(x)]}{\sum_{x \in d_X} \pi(x)}$$

where:

- $h = A(d)$;
- f - true dependency;

In most practical cases, $\mathrm{Err} \approx \mathrm{accuracy}.$

No free lunch, strictly

For any two learning algorithms A_1 and A_2:

1. uniformly averaged over all f, for any n:

$$\mathbb{E}(\mathrm{Err} \mid f, |D| = n, A_1) - \mathbb{E}(\mathrm{Err} \mid f, |D| = n, A_1) = 0$$

2. uniformly averaged over all f, for any d:

$$\mathbb{E}(\mathrm{Err} \mid f, d, A_1) - \mathbb{E}(\mathrm{Err} \mid f, d, A_1) = 0$$

3. uniformly averaged over all priors $P(f)$:

$$\mathbb{E}(\mathrm{Err} \mid |D| = n, A_1) - \mathbb{E}(\mathrm{Err} \mid |D| = n, A_1) = 0$$

4. uniformly averaged over all priors $P(f)$, for any d:

$$\mathbb{E}(\mathrm{Err} \mid d, A_1) - \mathbb{E}(\mathrm{Err} \mid d, A_1) = 0$$

No free lunch theorem

No free lunch theorem states that **on average by all datasets** all learning algorithms are equally bad at learning.
Examples:

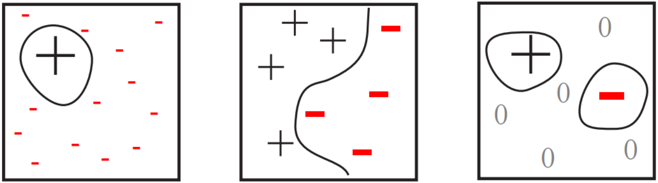
- crazy algorithm:

$$f(x) = \left\lfloor \left(\left\lceil \sum_i x_i + \theta \right\rceil \mod 17 + 1027 \right)^{\pi} \right\rfloor \mod 2$$

- any configuration of SVM

perform equally well **on average**.

No free lunch theorem



Possible learning algorithm behaviours in **problem space**:

- **+** - better than the average;
- — - worse than the average.

Is Machine Learning useless?

Is Machine Learning useless?

No.

Assumptions and algorithms

Is Machine Learning useless?

No Free Lunch theorem applies to:

- one learning algorithm;
- against all possible problems.

In real world we have:

- **data scientist** with prior knowledge of the world;
- problem description;
- data description;
- a set of standard algorithms.

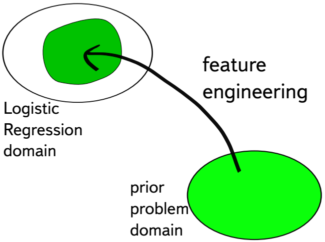
Is Machine Learning useless?

Real world problems often behave nicely:

- data is collected by humans (features are determined by humans);
    - algorithms with human-bias dominate (e.g. XGboost);
- problems are posed by humans;
- a lot of assumptions behind the data can be quickly identified from the problem domain.

Traditional ML (simplified)

- analyze the problem and make assumptions;
- pick an algorithm from a toolkit (e.g. logistic regression);
- provide assumptions suitable for the algorithm (**feature engineering**).



Discussion

- this approach works well for traditional datasets with a small number of features:
- e.g. Titanic dataset:

passenger class	name	gender	age	fare	...

Essentially, performance of the algorithm depends on:

- knowledge of the domain;
- feature engineering skills;
- understanding of assumptions behind standard algorithms.

Discussion

What are the assumptions behind:

- logistic regression,
- decision trees,
- linear SVM,
- SVM with RBF kernel?

Discussion

What about:

- cross-validation-based algorithm selection?

What if we consider accuracy instead of off-training-set accuracy?

What if we consider accuracy instead of off-training-set accuracy?

$$\text{accuracy} = \text{generalization} + \text{memorization}$$

What about other losses?

Representation matters

x_1	x_2	x_3	y
0	0	0	0
0	0	1	0
0	1	0	1
0	1	1	0
1	0	0	0
1	0	1	1
1	1	0	0
1	1	1	0

Representation matters

x_1	x_2	x_3	y
0	0	0	0
0	0	1	0
0	1	0	1
0	1	1	0
1	0	0	0
1	0	1	1
1	1	0	0
1	1	1	0

$$x = 4 \cdot x_1 + 2 \cdot x_2 + x_3$$

x	y
0	0
1	0
2	1
3	0
4	0
5	1
6	0
7	0

$$y = \begin{cases} 1, & x \mod 3 = 2; \\ 0, & \text{otherwise} \end{cases}$$

Representation matters

Solve with a descent algorithm:

$$(x-8)^2 \to \min$$

where: $x \in \{0, 1, \ldots, 15\}$

- $\text{neighbors}(x) = x \pm 1$;
- $\text{neighbors}(x) = \{z \mid \|\text{binary}(x) - \text{binary}(z)\|_1 = 1\}$

Algorithms

What makes a good family of learning algorithms (ML library)?

Corollary from No-Free-Lunch

A good machine learning family of algorithms/framework:

- has clear relation between hyperparameters and set of problems each algorithm covers.

A great machine learning family/frameworks:

- covers a wide range of problems;
- but each algorithm covers a small set of problems;
- i.e. a lot of sensitive and well-defined hyperparameters.

Here feature engineering/selection/generation is a part of the algorithm.

I just leave it here

Website | Documentation | Installation

build passing pypi package 0.1.1.9

CatBoost is a machine learning method based on gradient boosting over

Main advantages of CatBoost:

- Superior quality when compared with other libraries.
- Support for both numerical and categorical features.

Summary

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No-Free-Lunch:

- learning is impossible without prior knowledge;
- there is no silver bullet for learning;
- every learning algorithm has assumptions behind it;
- **data scientist's** job is to select/make an algorithm to match the assumptions.

References

No-Free-Lunch theorem:

- Schaffer, Cullen. ”A conservation law for generalization performance.” Proceedings of the 11th international conference on machine learning. 1994.
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- Wolpert, David H., and William G. Macready. ”No free lunch theorems for optimization.” IEEE transactions on evolutionary computation 1.1 (1997): 67-82.