CS 6316 Machine Learning

Model Selection and Validation

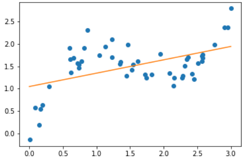
Yangfeng Ji

Department of Computer Science
University of Virginia

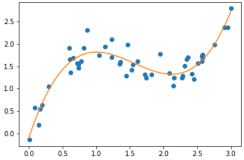
UNIVERSITY of VIRGINIA | ENGINEERING

Overview

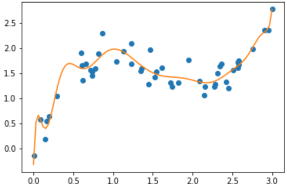
Polynomial regression



(a) $d = 1$



(b) $d = 3$

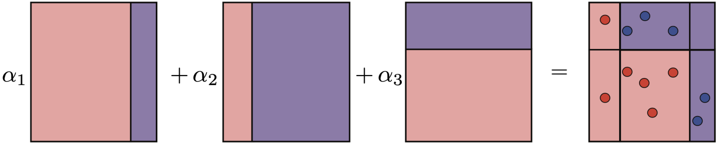


(c) $d = 15$

Boosting

Adaboost combines T weak classifiers to form a (strong) classifier

$$\text{sign}\left(\sum_{t=1}^{T} w_t h_t(\boldsymbol{x})\right) = h(\boldsymbol{x}) \tag{1}$$



where T controls the model complexity

[Mohri et al., 2018, Page 147]

Structural Risk Minimization

Take linear regression with ℓ_2 as an example. Let $\mathscr{H}_\lambda$ represents the hypothesis space defined with the following objective function

$$L_{S,\ell_2}(h_{\boldsymbol{w}}) = \frac{1}{m}\sum_{i=1}^{m}(h_{\boldsymbol{w}}(\boldsymbol{x}_i) - y_i)^2 + \lambda\|\boldsymbol{w}\|^2 \tag{2}$$

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- Another example: Support Vector Machines (next lecture)

Model Evaluation and Selection

Since we cannot compute the true error of any given hypothesis $h \in \mathcal{H}$

- How to evaluate the performance for a given model?
- How to select the best model among a few candidates?

Model Validation

Validation Set

The simplest way to estimate the true error of a predictor h

- Independently sample an additional set of examples V with size m_v

$$V = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_{m_v}, y_{m_v})\} \tag{3}$$

- Evaluate the predictor h on this validation set

$$L_V(h) = \frac{|\{i \in [m_v] : h(\boldsymbol{x}) \neq y_i\}|}{m_v}. \tag{4}$$

Usually, $L_V(h)$ is a good approximation to $L_{\mathcal{D}}(h)$

Theorem

Let h be some predictor and assume that the loss function is in $[0, 1]$. Then, for every $\delta \in (0, 1)$, with probability of at least $1 - \delta$ over the choice of a validation set V of size m_v, we have

$$|L_V(h) - L_{\mathcal{D}}(h)| \leq \sqrt{\frac{\log(2/\delta)}{2m_v}} \tag{5}$$

where

- $L_V(h)$: the validation error
- $L_{\mathcal{D}}(h)$: the true error

[Shalev-Shwartz and Ben-David, 2014, Theorem 11.1]

Sample Complexity

- The fundamental theorem of learning

$$L_{\mathscr{D}}(h) \leq L_S(h) + \sqrt{C\frac{d + \log(1/\delta)}{m}} \tag{6}$$

where d is the VC dimension of the corresponding hypothesis space

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  where d is the VC dimension of the corresponding hypothesis space
- On the other hand, from the previous theorem

$$L_{\mathcal{D}}(h) \leq L_V(h) + \sqrt{\frac{\log(2/\delta)}{2m_v}} \tag{7}$$

- A good validation set should have similar number of examples as in the training set

Model Selection

Model Selection Procedure

Given the training set S and the validation set V

- For each model configuration c, find the best hypothesis $h_c(\boldsymbol{x}, S)$

$$h_c(\boldsymbol{x}, S) = \underset{h' \in \mathcal{H}_c}{\operatorname{argmin}} \, L_S(h'(\boldsymbol{x}, S)) \tag{8}$$

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- With a collection of best models with different configurations $\mathcal{H}' = \{h_{c_1}(\boldsymbol{x}, S), \ldots, h_{c_k}(\boldsymbol{x}, S)\}$, find the overall best hypothesis

$$h(\boldsymbol{x}, S) = \operatorname*{argmin}_{h' \in \mathcal{H}'} L_V(h'(\boldsymbol{x}, S)) \tag{9}$$

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- It is similar to learn with the finite hypothesis space $\mathcal{H}'$

Model Configuration/Hyperparameters

Consider polynomial regression

$$\mathcal{H}_d = \{w_0 + w_1 x + \cdots + w_d x^d : w_0, w_1, \ldots, w_d \in \mathbb{R}\} \quad (10)$$

- the degree of polynomials d
- regularization coefficient λ as in $\lambda \cdot \|\boldsymbol{w}\|_2^2$
- the bias term w_0

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Additional factors during learning

- Optimization methods
- Dimensionality of inputs, etc.

Limitation of Keeping a Validation Set

If the validation set is

- small, then it could be biased and could not give a good approximation to the true error
- large, e.g., the same order of the training set, then we waste the information if do not use the examples for training.

k-Fold Cross Validation

The basic procedure of k-fold cross validation:

- Split the whole data set into k parts

Data

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Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

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- Take the average of k validation errors as the model error

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Cross-Validation Algorithm

Input: (1) training set S; (2) set of parameter values Θ; (3) learning algorithm A, and (4) integer k
Partition S into $S_1, S_2, \ldots, S_k$
for $\theta \in \Theta$ **do**
  for $i = 1, \ldots, k$ **do**
    $h_{i,\theta} = A(S \backslash S_i; \theta)$
  end for
  $\mathrm{Err}(\theta) = \frac{1}{k} \sum_{i=1}^{k} L_{S_i}(h_{i,\theta})$
end for
Output: the hypothesis $h_S(\boldsymbol{x}) = \mathrm{sign}(\sum_{t=1}^{T} w_t h_t(\boldsymbol{x}))$

In practice, k is usually 5 or 10.

Train-Validation-Test Split

- Training set: used for learning with a pre-selected hypothesis space, such as
  - logistic regression for classification
  - polynomial regression with $d = 15$ and $\lambda = 0.1$
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Typical splits on *all* available data

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Model Selection in Practice

What To Do If A Learning Fails

There are many elements that can help fix the learning procedure

- Get a larger sample

[Shalev-Shwartz and Ben-David, 2014, Page 151]

What To Do If A Learning Fails

There are many elements that can help fix the learning procedure

- Get a larger sample
- Change the hypothesis class by
  - Enlarging it
  - Reducing it
  - Completely changing it
  - Changing the parameters you consider

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- Change the feature representation of the data (usually domain dependent)
- Change the optimization algorithm used to apply your learning rule (lecture on optimization methods)

[Shalev-Shwartz and Ben-David, 2014, Page 151]

Error Decomposition Using Validation

With two additional terms

- $L_V(h_S)$: validation error
- $L_S(h_S)$: empirical (*or* training) error

the true error of h_S can be decomposed as

$$L_{\mathcal{D}}(h_S) = \underbrace{(L_{\mathcal{D}}(h_S) - L_V(h_S))}_{(1)} + \underbrace{(L_V(h_S) - L_S(h_S))}_{(2)} + \underbrace{L_S(h_S)}_{(3)}$$

- Item (1) is bounded by the previous theorem
- Item (2) is large: **overfitting**
- Item (3) is large: **underfitting**

About Large $L_S(h_S)$

Recall that h_S is an ERM hypothesis, aka

$$h_S \in \operatorname*{argmin}_{h' \in \mathcal{H}} L_S(h') \tag{11}$$

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Q: How to distinguish these two?

A: Find an existing simple baseline model

About Large $L_V(h_S)$

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3. the hypothesis space is inappropriate

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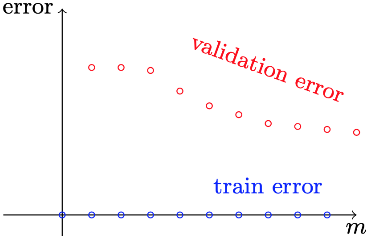
Comments

- Issue 1 and 2 are easy to fix
  - Get more data if possible, or reduce the hypothesis space
- How to distinguish issue 3 from 1 and 2?

Learning Curves

With different proportions of training examples, we can plot the training and validation errors



(a)

Figure: Examples of learning curves [Shalev-Shwartz and Ben-David, 2014, Page 153].

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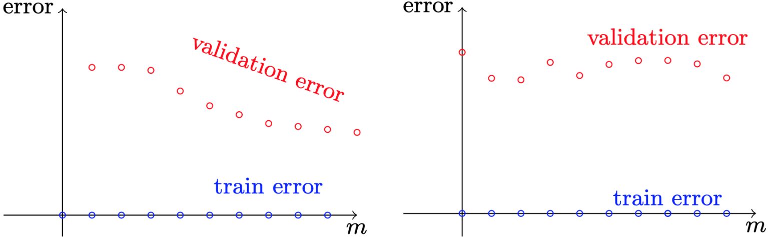

(a) (b)

Figure: Examples of learning curves [Shalev-Shwartz and Ben-David, 2014, Page 153].

Reference

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