HUST

ĐẠI HỌC BÁCH KHOA HÀ NỘI

HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

ONE LOVE. ONE FUTURE.

ĐẠI HỌC
BÁCH KHOA HÀ NỘI
HANOI UNIVERSITY
OF SCIENCE AND TECHNOLOGY

Machine Learning

IT3190E

Lecture: Performance evaluation

ONE LOVE. ONE FUTURE.

Contents

- Lecture 1: Introduction to Machine Learning
- Lecture 2: Linear regression
- Lecture 3+4: Clustering
- Lecture 5: Decision tree and Random forest
- Lecture 6: Neural networks
- Lecture 7: Support vector machines
- **Lecture 8: Performance evaluation**
- Lecture 9: Probabilistic models
- Lecture 10: Ensemble learning
- Lecture 11: Reinforcement learning
- Lecture 12: Regularization
- Lecture 13: Discussion on some advanced topics

1. Assessing performance (1)

- *How can we make a reliable assessment on the performance of an ML method?* (Làm thế nào để thu được một đánh giá đáng tin cậy về hiệu năng của một phương pháp ML?)
  - Note that performance of a method often improves as more data are available.
  - An assessment is more reliable as more data are used to test prediction.
- *How to choose a good value for a parameter in an ML method?* (Làm thế nào để lựa chọn tốt các tham số cho một phương pháp học máy?)
- The performance of a method depends on many factors:
  - Data distribution
  - Training size
  - Representativeness of training data over the whole space,…

Assessing performance (2)

- *Theoretical evaluation:* study some theoretical properties of a method/model with some explicit mathematical proofs.
  - Learning rate?
  - How many training instances are enough?
  - What is the expected accuracy of prediction?
  - Noise-resistance? …
- *Experimental evaluation:* observe the performance of a method in practical situations, using some datasets and a performance measure. Then make a summary from those experiments.
  (Quan sát hệ thống làm việc trong thực tế, sử dụng một hoặc nhiều tập dữ liệu và các tiêu chí đánh giá. Tổng hợp đánh giá từ các quan sát đó.)
- We will discuss experimental evaluation in this lecture.

Assessing performance (3)

- ***Model assessment:*** *we need to evaluate the performance of a method/model, only based on a given observed dataset D.*
  (cần đánh giá hiệu năng của phương pháp (model) A, chỉ dựa trên bộ dữ liệu đã quan sát D.)
- Evaluation:
  - Should be done automatically,
  - Does not need any help from users.
- Evaluation strategies:
  - To obtain a reliable assessment on performance.
- Evaluation measures:
  - To measure performance quantitatively.

2. Some evaluation techniques

- Hold-out
- Stratified sampling
- Repeated hold-out
- Cross-validation
  - K-fold
  - Leave-one-out
- Bootstrap sampling

Hold-out (random splitting)

- The observed dataset D is randomly splitted into 2 non-overlapping subsets:
  - D_{train}: used for training
  - D_{test}: used to test performance

- Note that:
  - No instance of D_{test} is used in the training phase.
  - No instance of D_{train} is used in the test phase.
- Popular split: $|D_{train}| = (2/3).|D|$, $|D_{test}| = (1/3).|D|$
- This technique is suitable when D is of large size.

Stratified sampling

- For small or imbalanced datasets, random splitting might result in a training dataset which are not representative.
  - A class in D_{train} might be empty or have few instances.
- *We should split D so that the class distribution in D_{train} is similar with that in D.*
- Stratified sampling fulfills this need:
  - *We randomly split each class of D into 2 parts:* one is for D_{train}, and the other is for D_{test}.
  - for each class:

- Note that this technique cannot be applied to regression and unsupervised learning.

Repeated hold-out

- We can do hold-out many times, and then take the average result.
  - Repeat hold-out n times. The i^{th} time will give a performance result p_i. The training data for each hold-out should be different from each other.
  - Take the average p = mean(p_1,…, p_n) as the final quality.
- Advantages?
- Limitations?

Cross-validation

- In repeated hold-out: there are overlapping between two training/testing datasets. It might be redundant.
- *K-fold cross-validation:*
  - *Split D into K equal parts which are non-overlapping.*
  - *Do K runs (folds): at each run, one part is used for testing and the remaining parts are used for training.*
  - *Take the average as the final quality from K individual runs.*

- Popular choices of K: 10 or 5
- It is useful to combine this technique with stratified sampling.
- This technique is suitable for small/average datasets.

Leave-one-out cross-validation

- It is K-fold cross-validation when K = |D|.
  - Each testing set consists of only one instance from D.
  - The remaining is for training.
- So all observed instances are exploited as much as possible.
- No randomness appears.
- But it is expensive, and hence is suitable with small datasets.

Bootstrap sampling

- Previous methods do not allow repetitions of an instance in any training part.
- Bootstrap sampling:
  - Assume D having n instances.
  - Build D_{train} by randomly sampling (with replacement/repetition) n instances from D.
  - D_{train} is used for the training phase.
  - $D_{test} = D \backslash D_{train}$ is used for testing quality.
  - Note that $D_{test} = \{z \in D: z \notin D_{train}\}$
- It can be shown that D_{train} contains nearly 63.2% different instances of D. 36.8% of D are used for testing.
- This technique is suitable for small datasets.

3. Model selection

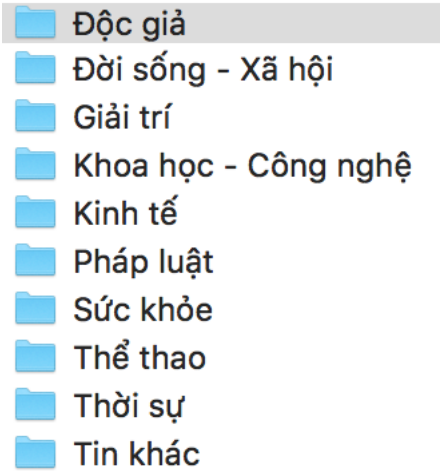
- An ML method often has a set of hyperparameters that require us to select suitable values a priori.
  - λ in Ridge regression; C in Linear SVM
- How to choose a good value?
- ***Model selection:*** *given a dataset D, we need to choose a good setting of the hyperparameters in method (model) A such that the function learned by A generalizes well.*
  (từ một tập học D, cần lựa chọn bộ tham số (model) trong phương pháp học A sao cho hệ thống được huấn luyện tốt nhất từ D.)
- A validation set T_{valid} is often used to find a good setting.
  - It is often a subset of D.
  - A good setting should help the learned function predicts well on T_{valid}.
    → we are approximating the generalization error on the whole data space by just using a small set T_{valid}.

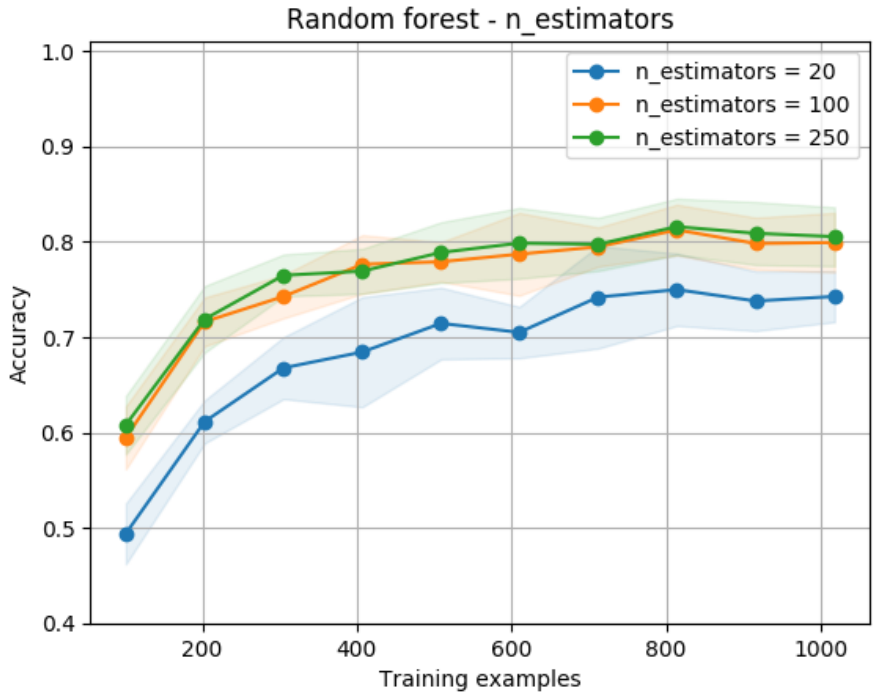
Model selection: using hold-out

- Given an observed dataset D, we can **select** a good value for hyperparamerter λ as follows:
  - *Select a finite set S which contains all potential values of λ.*
  - *Select a performance measure P.*
  - *Randomly split D into 2 non-overlapping subsets: D_{train} and T_{valid}*
  - *For each $\lambda \in S$: train the system given D_{train} and λ. Measure the quality on T_{valid} to get P_{λ}.*
  - *Select the best λ* which corresponds to the best P_{λ}.*
- It is often beneficial to learn again from D given λ* to get a better function.
- Hold-out can be replaced with other techniques e.g., sampling, cross-validation.

Example: select parameters

- Random forest for news classification
  - Parameter: n_estimates (number of trees)
- Dataset: *1135 news, 10 classes, vocabulary of 25199 terms*
- 10-fold cross-validation is used





4. Model assessment and selection

- Given an observed dataset D, we need to **select** a good value for hyperparamerter λ and **evaluate** the overall performance of a method A:
  - *Select a finite set S which contains all potential values of λ.*
  - *Select a performance measure P.*
  - *Split D into 3 non-overlapping subsets: D_{train}, T_{valid} and T_{test}*
  - *For each $\lambda \in S$: train the system given D_{train} and λ. Measure the quality on T_{valid} to get P_λ.*
  - *Select the best λ* which corresponds to the best P_λ.*
  - Train the system again from $D_{train} \cup T_{valid}$ given λ*.
  - Test performance of the system on T_{test}.
- Hold-out can be replaced with other techniques.

5. Performance measures

- Accuracy (độ chính xác)
  - Percentage of correct predictions on testing data.
- Efficiency (tính hiệu quả)
  - The cost in time and storage when learning/prediction.
- Robustness (khả năng chống nhiễu)
  - The ability to reduce possible affects by noises/errors/missings.
- Scalability (tính khả mở)
  - The relation between the performance and training size.
- Complexity (độ phức tạp)
  - The complexity of the learned function.
- …

Accuracy

- Classification:

$$Accuracy = \frac{number\ of\ correct\ predictions}{Total\ number\ of\ predictions}$$

- Regression: (MAE – mean absolute error)

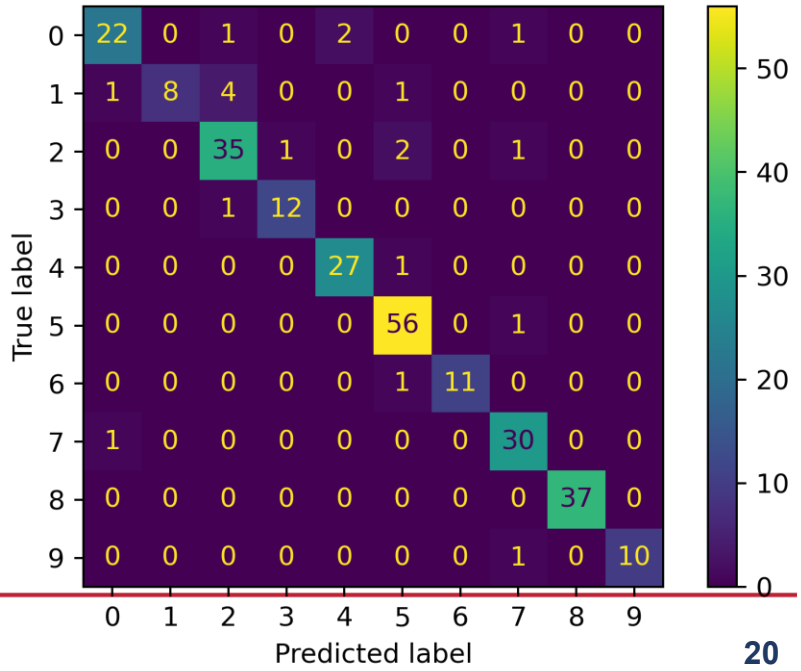
$$MAE = \frac{1}{|D_{test}|} \sum_{x \in D_{test}} |o(x) - y(x)|$$

  - o(x) is the prediction for an instance x.
  - y(x) is the true value.

Confusion matrix

- (ma trận nhầm lẫn) Can help us see predictions for each class in details
- Multiclass classification
  - *TP_i (true possitive):* the number of instances that are assigned correctly to class c_i.
  - *FP_i (false possitive):* the number of instances that are assigned incorrectly to class c_i.
  - *FN_i (false negative):* the number of instances inside c_i that are assigned incorrectly to another class.

	Predicted label		
True label	TP_1	FN_{12}	FN_{13}
	FP_{21}	TP_2	FN_{23}
	FP_{31}	FP_{32}	TP_3



Precision and Recall (1)

- These two measures are often used for classification
- **Precision** for class c_i:
  - Percentage of correct instances, among all that are assigned to c_i.

$$Precision(c_i) = \frac{TP_i}{TP_i + FP_i}$$

- **Recall** for class c_i:
  - Percentage of instances in c_i that are correctly assigned to c_i.

$$Recall(c_i) = \frac{TP_i}{TP_i + FN_i}$$

Precision and Recall (2)

- To give an overall summary, we can take an average from individual classes.
- Micro-averaging: (chất lượng trung bình cho từng phán đoán)

$$Precision = \frac{\sum_{i=1}^{|C|} TP_i}{\sum_{i=1}^{|C|} (TP_i + FP_i)} \qquad Recall = \frac{\sum_{i=1}^{|C|} TP_i}{\sum_{i=1}^{|C|} (TP_i + FN_i)}$$

- Macro-averaging: (chất lượng trung bình cho từng lớp)

$$Precision = \frac{\sum_{i=1}^{|C|} Precision(c_i)}{|C|} \qquad Recall = \frac{\sum_{i=1}^{|C|} Recall(c_i)}{|C|}$$

F_1

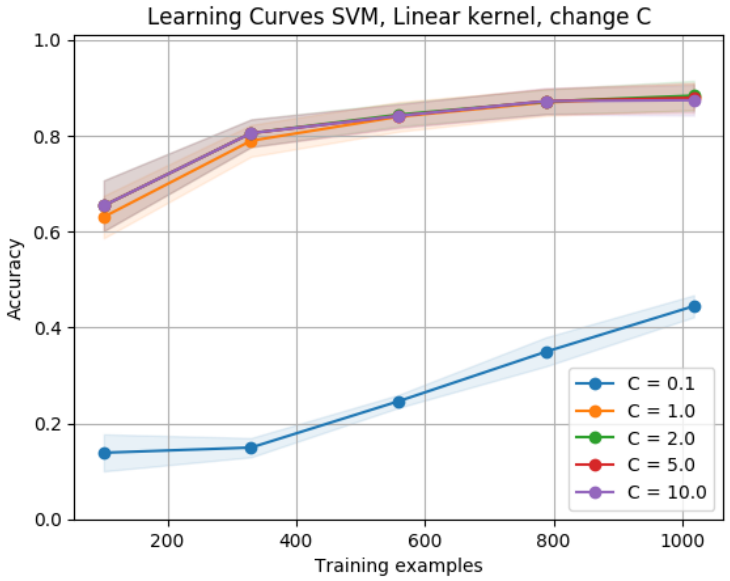
- Precision and recall provide us different views on the performance of a classifier.
- F_1 can provide us a unified view.
- F_1 is the *harmonic mean* of precision and recall, and is computed as:

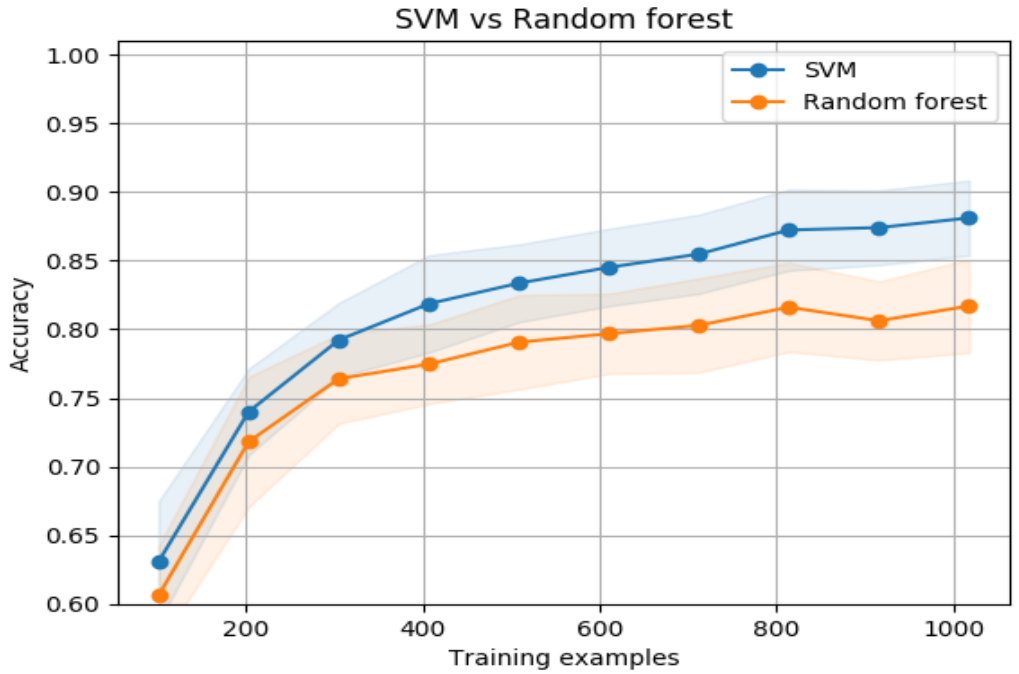
$$F_1 = \frac{2.Precision.Recall}{Precision + Recall} = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}}$$

  - F_1 tends to be close to the smaller value from {precision, recall}
  - Large F_1 implies that both precision and recall are large.

Example: compare 2 methods

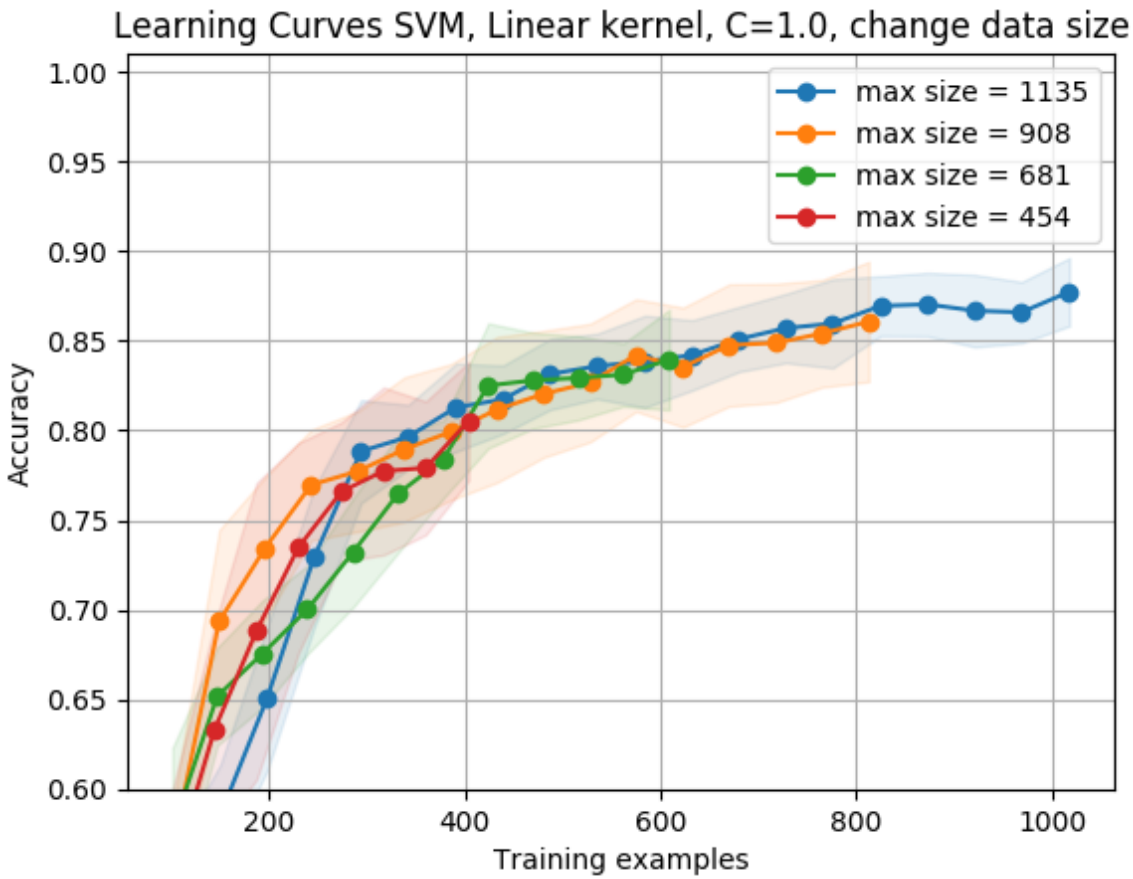
- Methods: **Random forest** vs **Support vector machines** (SVM)
- Parameter selection: 10-fold cross-validation
  - Random forest: n_estimate = 250
  - SVM: regularization constant C = 1





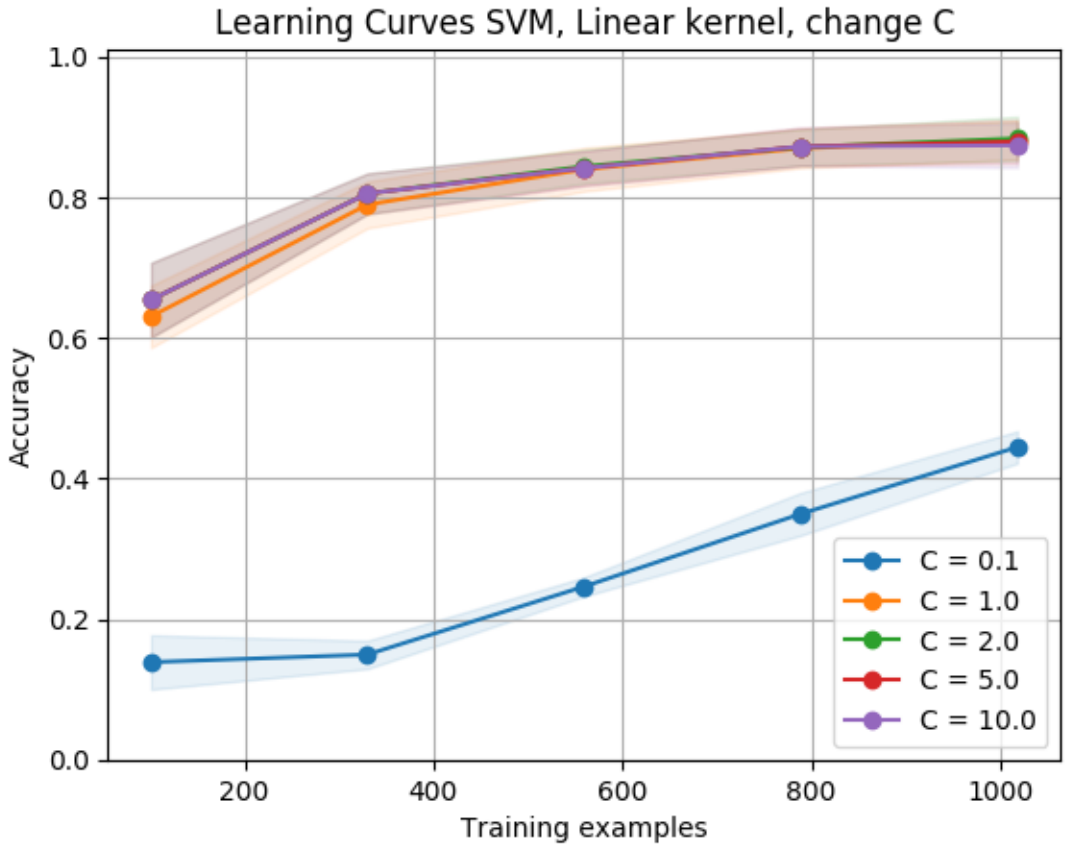
Example: effect of data size

- SVM
  - Parameter: size of training data
- Dataset: *1135 news, 10 classes, vocabulary of 25199 terms*
- 10-fold cross-validation is used



Example: effect of parameters

- SVM for news classification
  - Parameter C changes
- Dataset: *1135 news, 10 classes, vocabulary of 25199 terms*
- 10-fold cross-validation is used



References

- Trevor Hastie, Robert Tibshirani, Jerome Friedman. *The Elements of Statistical Learning*. Springer, 2009.
- Sebastiani, F. (2002). Machine learning in automated text categorization. *ACM computing surveys (CSUR)*, *34*(1), 1-47.

HUST

hust.edu.vn fb.com/dhbkhn

THANK YOU !