Introduction to

Machine Learning and Data Mining

(Học máy và Khai phá dữ liệu)

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Contents

1. Assessing performance (1)

- *How can we make a reliable assessment on the performance of an ML method?*
  - 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?*
- The performance of a method depends on many factors:
  - Class 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.
- 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.*
- 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: D_{train} D_{test}
- 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 $p = mean(p_1,\ldots, p_n)$ 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.
  - Ridge regression: λ
  - Linear SVM: C
- 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.*
- A validation set T_{valid} is often used to find a good setting.
  - It is a subset of D.
  - A good setting should help the learned function predicts well on T_{valid}.

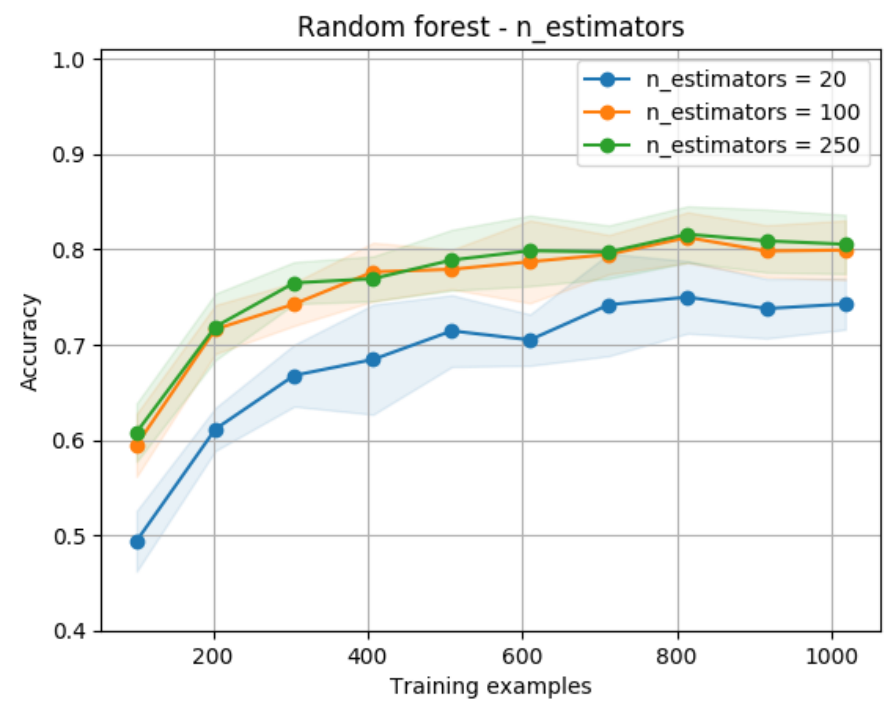
Model selection: using hold-out

- 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

Độc giả
Đời sống - Xã hội
Giải trí
Khoa học - Công nghệ
Kinh tế
Pháp luật
Sức khỏe
Thể thao
Thời sự
Tin khác



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:
  - Percentage of correct predictions on testing data.
- Efficiency:
  - The cost in time and storage when learning/prediction.
- Robustness:
  - The ability to reduce possible affects by noises/errors/missings.
- Scalability:
  - The relation between the performance and training size.
- Complexity:
  - The comlexity 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.

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.

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

- *TP_i*: the number of instances that are assigned correctly to class c_i.
- *FP_i*: the number of instances that are assigned incorrectly to class c_i.
- *FN_i*: the number of instances inside c_i that are assigned incorrectly to another class.
- *TN_i*: the number of instances outside c_i that are not assigned to class c_i.

Precision and Recall (1)

- These two measures are often used in information retrieval and 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:

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

- Macro-averaging:

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

F_1

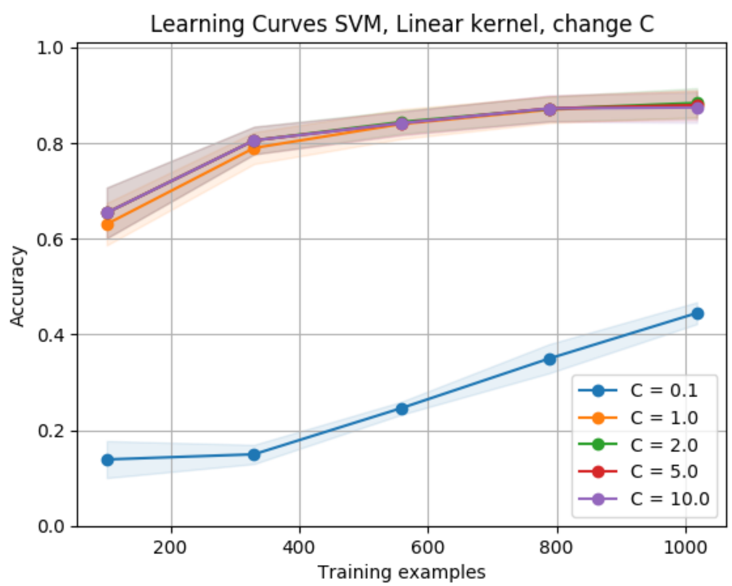
- Precision and recall provide us different views on the performance of a classifier.
- F_1 can provide us a unified view.
- F_1 is the *harmonic mean* of precision and recall, and is computed as:

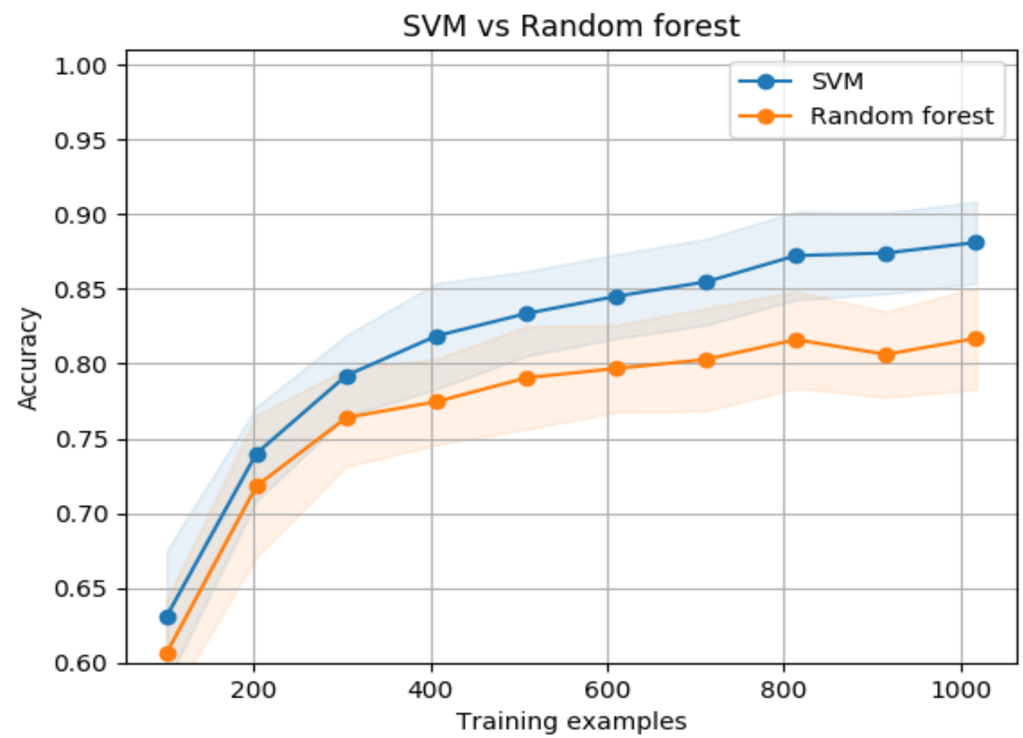
$$F_1 = \frac{2.Precision.Recall}{Precision + Recall} = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}}$$

  - 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

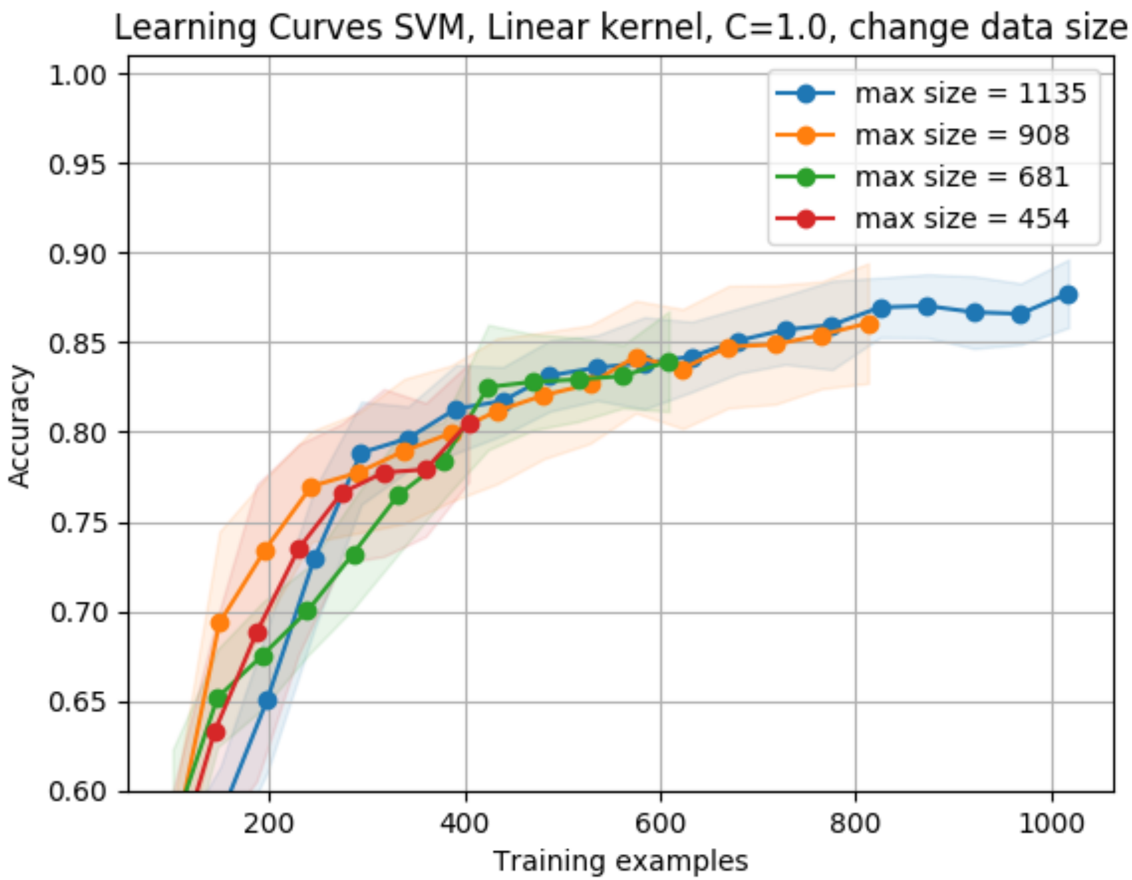
- Methods: **Random forest** vs **Support vector machines** (SVM)
- Parameter selection: 10-fold cross-validation
  - Random forest: n_estimate = 250
  - SVM: regularization constant C = 1





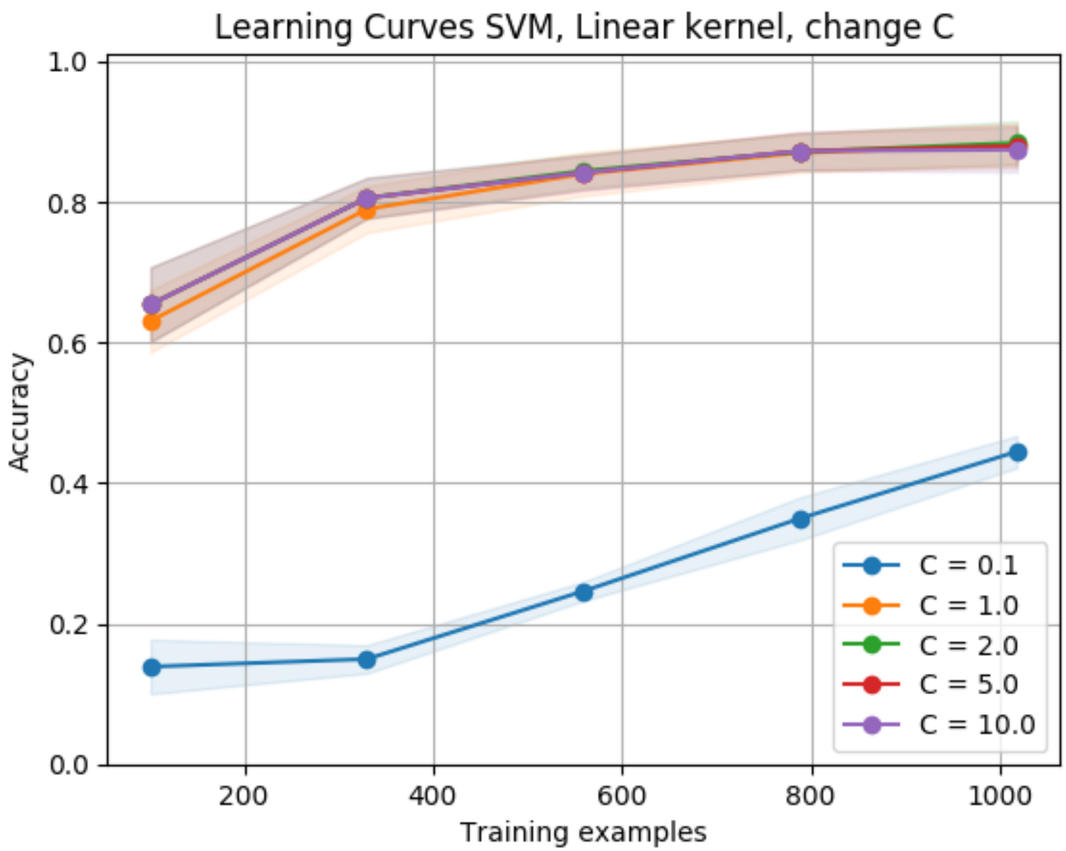
Example: effect of data size

- 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



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