

程序代写代做 CS编程辅导



Data Splitting Bias-Variance Tradeoff

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# Supervised v. Unsupervised Learning

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- Machine learning is divided into **supervised** and **unsupervised** learning problems
- Supervised is further divided into **regression** and **classification**
- A core problem in machine learning is that the learning process tends to **overfit** to the training data, and therefore makes poor test and out-of-sample predictions

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# Definition of Bias-Variance Tradeoff

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- **Bias:** The difference between a model's prediction and the actual value of an observation
- **Variance:** The complexity of the model

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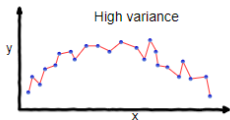
$$Err(x) = Bias^2 + Variance + \epsilon$$

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# Overfitting Visual Intuition

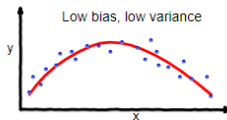
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overfitting



underfitting



Good balance

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Figure 1: Over and Underfitting

# Machine Learning

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- Develop dynamic models that are data-dependent
- Basic Process:
  - Split data into **training**, **validation**, and **test** sets
  - Train the ML algorithm
  - Use the validation set to make adjustments to the model(s)
  - Test the final model on the test set
  - Operationalize algorithm on new data

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# Machine Learning

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- Supervised Learning
  - Training data contains *labels* for the outcomes
  - Machine Learning algorithm infers a function describing the relationship between the inputs and the output
  - Algorithm can be used on a new set of input data to infer the output
  - Examples: Linear Regression, Decision Trees, Support Vector Machines, etc.
- Unsupervised Learning
  - Training data does not contain any labels
  - Algorithm instead tries to uncover underlying patterns in the data
  - Used for clustering, dimensionality reduction, etc.
  - Examples: k-means, Principal Components Analysis, Singular Value Decomposition, Expectation-Maximization



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# Regression and Classification

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- Typically two tasks in supervised learning: regression and classification
- Regression
  - Predict a continuous outcome response from the input data
  - Ex. Ordinary Least Squares
- Classification
  - Predict membership in a group
  - Ex. Logistic Regression
- Several ML methods are well suited to both regression and classification problems
- An important first step in any supervised machine learning problem is to identify whether you're dealing with a regression or classification problem, and approach it accordingly

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# Bias-Variance Tradeoff

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- Two goals:
  - Minimize *test bias*: This means using as much data as we can in the training phase, which necessarily means reducing the amount of test data available
  - Minimize *test variance*: But, we also want a decent number of points in the test set, otherwise the estimates will have large variances
- Fewer folds lead to higher test bias, but more folds lead to higher test variance

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# Cross-Validation

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- Introduced to statistics from machine learning
- Procedure for k-fold:
  - Partition the data into a number of folds
  - Train the data on  $k-1$  folds
  - Test on the last fold
  - Rotate so that the  $i$ th fold acts as the test set once
  - Take the mean estimate

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# Cross-Validation

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- Advantages:
  - Tends to avoid overfitting problems
  - Usable with small datasets (compared to train/test/validation split)
  - Does not make the background assumptions required in information criteria approach
- Disadvantages:
  - Assumes that the out-of-sample data was drawn from the same population as the training data
  - Computationally VERY expensive
- $k=5$  or  $10$  is conventionally used, but it is by no means perfectly suited to every context
- In general, this problem lessens the more data you have

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# K-Fold CV Illustration

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**Figure 2:** Illustration of k-fold cross validation

# Cross-Validation Techniques

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- K-Fold
  - Divide into k-folds and rotate
- Leave-one-out (LOO)
  - Leave out one observation, train the model on the rest, and calculate on the left out observations.

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# Comparison

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- Cross-Validation is generally preferred nowadays because of advances in computing.
- However, AIC is asymptotically equivalent to LOOCV if the assumptions are met.
- Generally use cross-validation unless it is computationally cost prohibitive.

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## Conclusion

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- Machine Learning requires we split our data to evaluate our models
- Data splitting involves substantive choices on the part of the analyst
- Different techniques have different pros and cons, but the main issue comes down to bias-variance tradeoff

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