CSC411/2515 Tutorial: K-NN and Decision Tree

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Cross-validation

K-nearest-neighbours

Decision Trees

Review: Motivation for Validation

Framework:	learning as optimization
Goal:	optimize model complexity (for our task)
Formulation:	minimize underfitting and overfitting

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Formulation: minimize underfitting and overfitting

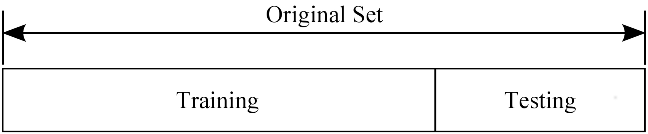
In particular, we want our model to generalize well without overfitting.

We can ensure this by validating the model.

Types of Validation (1)

hold-out validation: split data into training set and validation set

- usually: 30% as hold-out set



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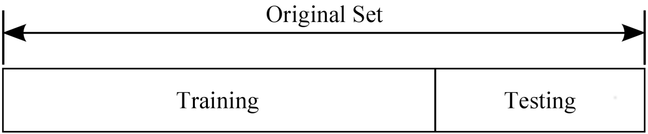
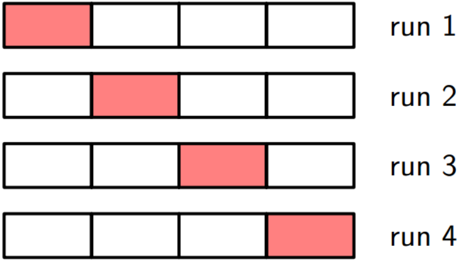


Problems:

- waste of dataset
- estimation of error rate may be misleading

Types of Validation (2)

cross-validation: random sub-sampling



[1]

[1] Figure from Bishop, C. M. (2006). *Pattern Recognition and Machine Learning*. Springer.

Types of Validation (2)

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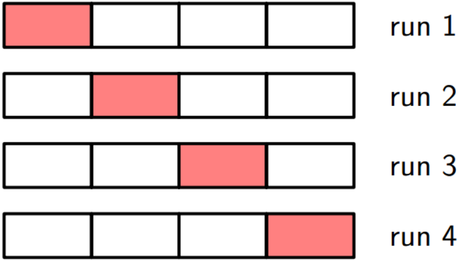

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Problem:

- more computationally expensive than *hold-out* validation

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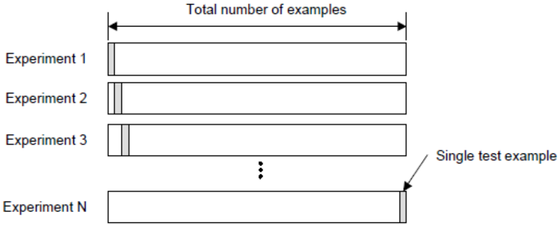
Variants of Cross-validation (1)

leave-p-out: use p examples as the validation set, and the rest as training; repeat for all configurations of examples.

e.g., for $p = 1$:



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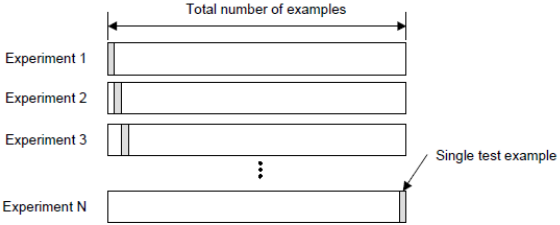
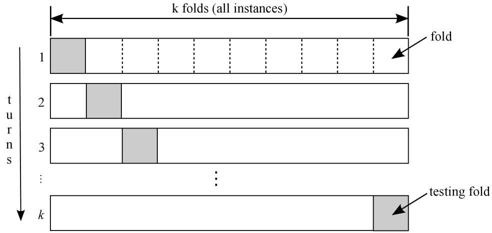


Problem:

- exhaustive: We are required to train and test $\binom{N}{p}$ times, where N is the number of training examples.

Variants of Cross-validation (2)

K-fold: partition training data into K equally sized subsamples; for each fold, use $K-1$ subsamples as training data with the last subsample as validation



Variants of Cross-validation (2): K-fold

Advantages:

- All observations are used for both training and validation, and each observation is used for validation exactly once.
- non-exhaustive $\implies$ more tractable than LpOCV

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Problems:

- expensive for large N, K (since we train/test K models on N examples)
  - but there are some efficient hacks to save time over the brute-force method . . .
- can still overfit if we validate too many models!
  - **Solution**: hold out an additional test set before doing any model selection, and check that the best model performs well even on the additional test set (*nested cross-validation*)

Practical Tips for Using K-fold Cross-validation

- **Q:** How many folds do we need?
- **A:** with larger K, ...
  - error estimation tends to be more accurate
  - but computation time will be greater

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In practice:

- usually choose $K \approx 10$
- BUT larger dataset $\Longrightarrow$ choose smaller K

Cross-validation

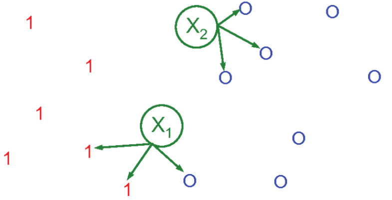
K-nearest-neighbours

Decision Trees

K-nearest-neighbours: Definition

Training: store all training examples (perfect memory)

Test: predict value/class of an unseen (test) instance based on closeness to stored training examples, relative to some distance (similarity) measure



[2]

[2] Figure from Murphy, K. P. (2012). *Machine Learning: A Probabilistic Perspective*. MIT press.

Predicting with K-nearest-neighbours

- for $K = 1$,
  - predict the same value/class as the nearest instance in the training set.
- for $K > 1$,
  - find the K closest training examples, and either
    - predict class by majority vote (in classification).
    - predict value by average weighted inverse distance (in regression).

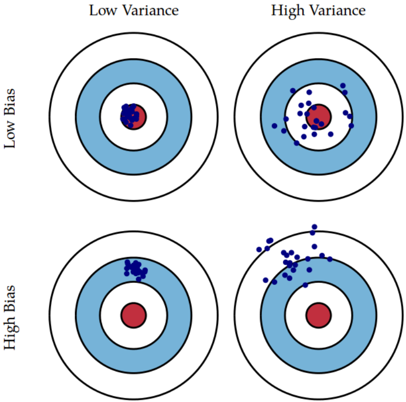
Practical Tips for Using KNN (1)

- ties may occur in a classification problem when $K > 1$
  - for binary classification: choose K odd to avoid ties
  - for multi-class classification:
    - decrease the value of K until the tie is broken
    - if that doesn't work, use the class given by a 1NN classifier

Practical Tips for Using KNN (2)

- magnitude of K:
    - smaller K: predictions have higher variance (less stable)
    - larger K: predictions have higher bias (less true)

Aside: The Bias-variance Tradeoff



A learning procedure creates biased models if . . .

- the predictive distribution of the models differs greatly from the target distribution.

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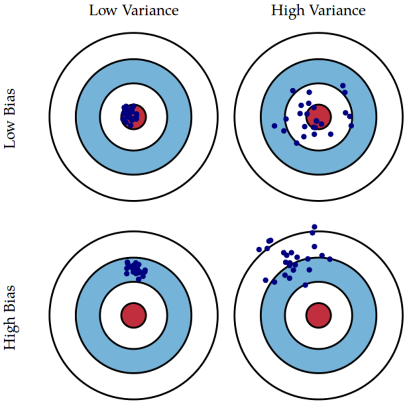

A learning procedure creates biased models if . . .

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A learning procedure creates models with high variance if . . .

- the models have greatly different test predictions (across different training sets from the same target distribution).

Practical Tips for Using KNN (2)

- magnitude of K:
  - smaller K: predictions have higher variance (less stable)
  - larger K: predictions have higher bias (less true)

Cross-validation can help here!

Practical Tips for Using KNN (3)

- the choice of distance measure affects the results!
  - e.g., standard Euclidean distance:

$$d_E(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_i (\mathbf{x}_i - \mathbf{y}_i)^2}$$

Problems:

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- in high-dimensional space, noisy features dominate
  - **Solution**: apply (learn?) feature weightings

Practical Tips for Using KNN (4)

- KNN has perfect memory, so computational complexity is an issue
  - at test time: $\mathcal{O}(N \cdot D)$ computations per test point

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Solutions:

- dimensionality reduction
  - sample features
  - project the data to a lower dimensional space
- sample training examples
- use clever data structures, like k-D trees

MATLAB Demo

Cross-validation

K-nearest-neighbours

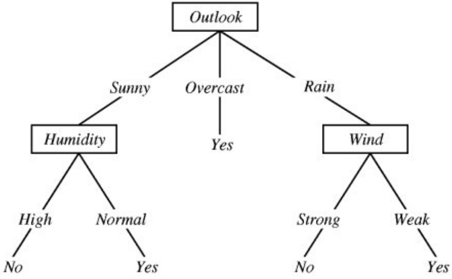
Decision Trees

Decision Trees: Definition

Goal: Approximate a discrete-valued target function

Representation: a tree, of which

- each internal (non-leaf) node tests an attribute
- each branch corresponds to an attribute value
- each leaf node assigns a class



[3]

[3] Example from Mitchell, T (1997). *Machine Learning*, McGraw Hill.

Decision Trees: Induction

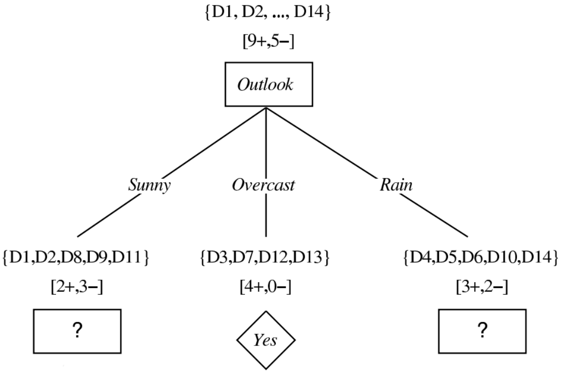
The ID3 algorithm:

- while training examples are not perfectly classified, do
  - choose the "most informative" attribute θ (that has not already been used) as the decision attribute for the next node N (greedy selection)
  - for each value (discrete θ) / range (continuous θ), create a new descendant of N
  - sort the training examples to the descendants of N

Decision Trees: Example *PlayTennis*

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

After splitting the training examples first on *Outlook* . . .



What should we choose as the next attribute under the branch *Outlook* = Sunny?

Choosing the "Most Informative" Attribute

Formulation: Maximise information gain over attributes Y.

Information Gain $(PlayTennis \mid Y)$

$$= H(PlayTennis) - H(PlayTennis \mid Y)$$

$$= \sum_x P(PlayTennis = x) \log P(PlayTennis = x)$$
$$- \sum_{x,y} P(PlayTennis = x, Y = y) \log \frac{P(Y = y)}{P(PlayTennis = x, Y = y)}$$

Information Gain Computation (1)

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
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$$\begin{aligned}\text{InfoGain}\,(\mathit{PlayTennis} \mid \text{Humidity}) &= .970 - \tfrac{3}{5}(0.0) - \tfrac{2}{5}(0.0) \\ &= .970\end{aligned}$$

Information Gain Computation (2)

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$$\begin{aligned}\text{InfoGain}\,(\textit{PlayTennis} \mid \text{Temperature}) &= .970 - \tfrac{2}{5}(0.0) - \tfrac{2}{5}(1.0) - \tfrac{1}{5}(0.0) \\ &= .570\end{aligned}$$

Information Gain Computation (3)

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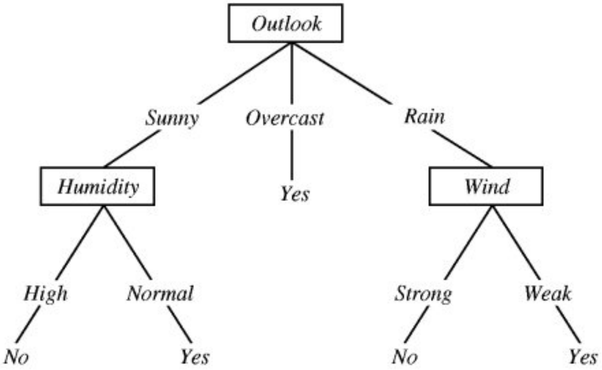
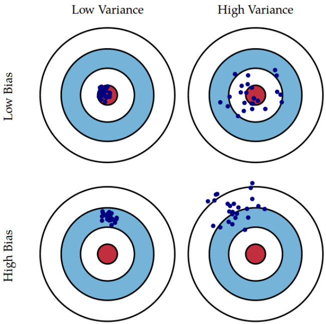
$$\begin{aligned} \text{InfoGain}\left(\textit{PlayTennis} \mid \text{Wind}\right) &= .970 - \tfrac{2}{5}(1.0) - \tfrac{3}{5}(0.918) \\ &= .019 \end{aligned}$$

The Decision Tree for *PlayTennis*

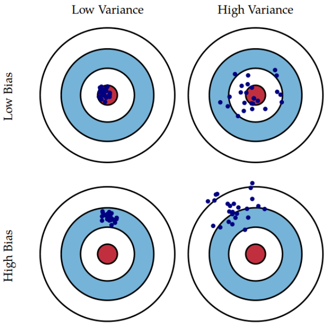


Recall: The Bias-variance Tradeoff



- Where do decision trees naturally lie in this space?

Recall: The Bias-variance Tradeoff



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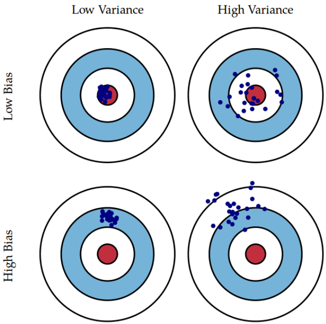

- Where do decision trees naturally lie in this space?
- **Answer**: high variance
- **How to fix**: pruning (e.g., *reduced-error* pruning, *rule post-pruning*)