Applied Machine Learning

Feature Selection: Wrapper Methods

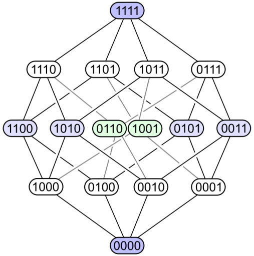
Learning goals

- Objective Functions
- Greedy Forward Search
- Greedy Backward Search

INTRODUCTION

- Wrapper methods emerge from the idea that different sets of features can be optimal for different learners
- Wrapper is a discrete search strategy for S, where objective criterion is test error of learner as function of S. Criterion can also be calculated on train set, approximating test error (AIC, BIC)

$\Rightarrow$ Use the learner to assess the quality of the feature sets



Hasse diagram illustrating search space. Knots are connected if Hamming distance = 1
(Source: Wikipedia)

OBJECTIVE FUNCTION

Given p features, **best-subset selection problem** is to find subset $S \subseteq \{1, \dots p\}$ optimizing objective $\Psi : \Omega \rightarrow \mathbb{R}$:

$$S^* \in \arg\min_{S \in \Omega} \{\Psi(S)\}$$

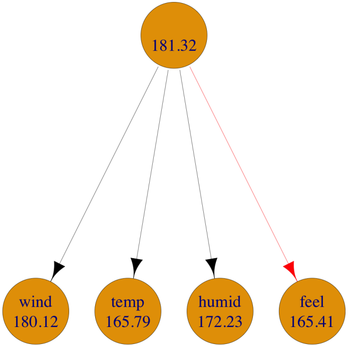
- Ω = search space of all feature subsets $S \subseteq \{1, \dots, p\}$. Usually we encode this by bit vectors, i.e., $\Omega = \{0, 1\}^p$ (1 = feat. selected)
- Objective Ψ can be different functions, e.g., AIC/BIC for LM or cross-validated performance of a learner
- Poses a discrete combinatorial optimization problem over search space of size = 2^p, i.e., grows exponentially in p (power set)
- Unfortunately can not be solved efficiently in general (NP hard; see, e.g., ▸ Natarajan 1995)
- Can avoid searching entire space by employing efficient search strategies, traversing search space in a “smart" way

GREEDY FORWARD SEARCH

Let $S \subset \{1, \ldots, p\}$ be subset of feature indices.

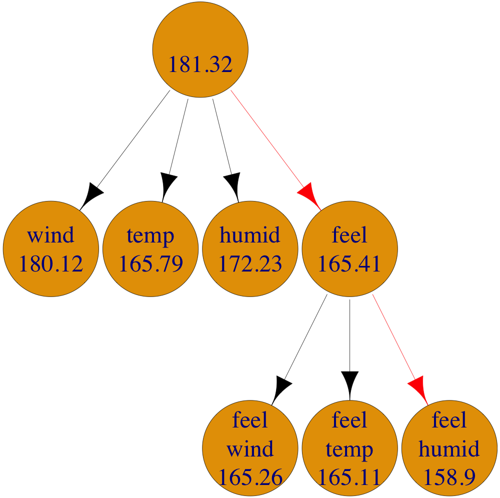
1. Start with the empty feature set $S = \emptyset$
2. For a given set S, generate all $S_j = S \cup \{j\}$ with $j \notin S$.
3. Evaluate the classifier on all S_j and use the best S_j

Example GFS on a subset of bike sharing data with features windspeed, temp., humidity and feeling temp. Node value is RMSE.



VISUALIZATION OF GFS

4. Iterate over this procedure



VISUALIZATION OF GFS

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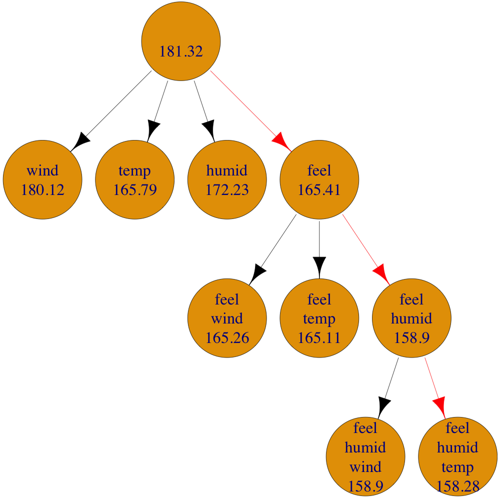
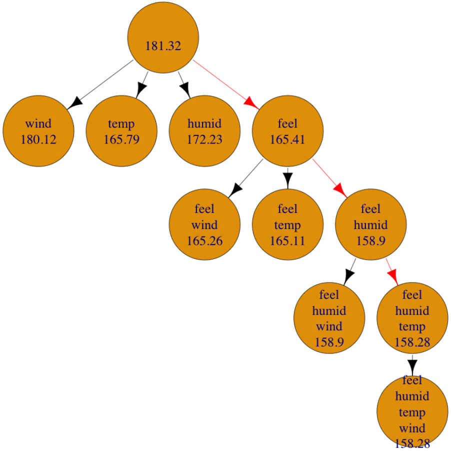


VISUALIZATION OF GFS



5. Terminate if performance does not improve further or max. number of features is used

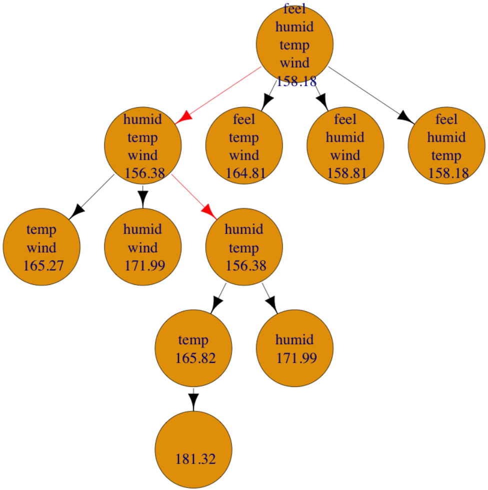
GREEDY BACKWARD SEARCH

- Start with the full index set of features $S = \{1, \ldots, p\}$.
- For a given set S generate all $S_j = S \setminus \{j\}$ with $j \in S$.
- Evaluate the classifier on all S_j and use the best S_j.
- Iterate over this procedure.
- Terminate if:
  - the performance drops drastically, or
  - falls below given threshold.

- GFS is much faster and generates sparser feature selections
- GBS much more costly and slower, but sometimes slightly better.

VISUALIZATION OF GBS

Example Greedy Backward Search on bike sharing data



ADVANTAGES AND DISADVANTAGES

Advantages

- Inducer-agnostic
- Any performance measure can be used
- Optimizes the desired performance measure directly

Disadvantages

- Expensive
- Does not scale well with the number of features
- Does (in general) not use additional info about model structure
- Nested resampling becomes necessary