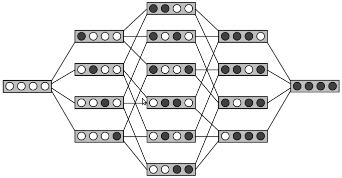
Introduction to Machine Learning

Feature Selection
Feature Selection: Wrapper methods



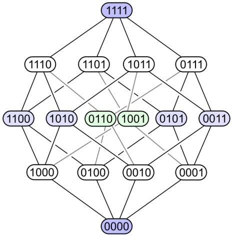
Learning goals

- Understand how wrapper methods work
- Forward + backward search, EAs
- Advantages and disadvantages

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

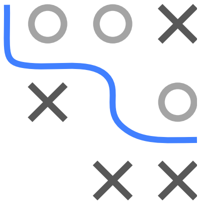


Hasse diagram illustrating search space. Knots are connected if Hamming distance = 1
(Source: Wikipedia)

OBJECTIVE FUNCTION

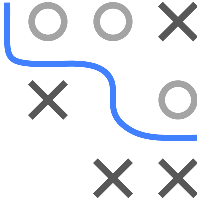
Given p features, **best-subset selection problem** is to find subset $S \subseteq \{1, \dots p\}$ optimizing objective $\Psi : \Omega \to \mathbb{R}$:

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



- 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

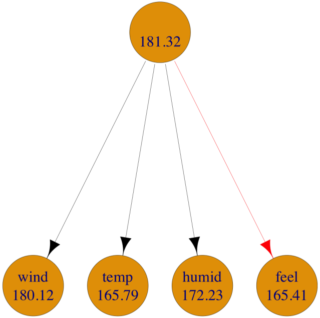
GREEDY FORWARD SEARCH



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

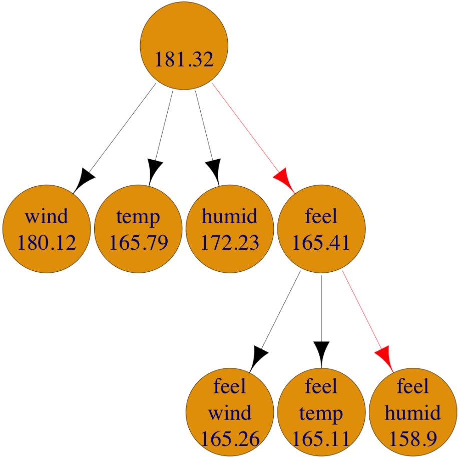
1. Start with the empty feature set $S = \emptyset$
2. For a given set S, generate all $S_j = S \cup \{j\}$ with $j \notin S$.
3. Evaluate the classifier on all S_j and use the best S_j

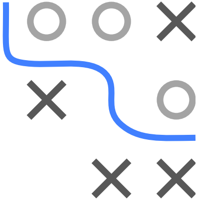
Example GFS on a subset of bike sharing data with features windspeed, temp., humidity and feeling temp. Node value is RMSE.



VISUALIZATION OF GFS

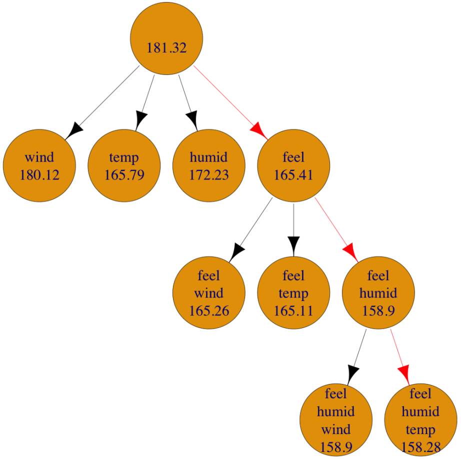
4. Iterate over this procedure

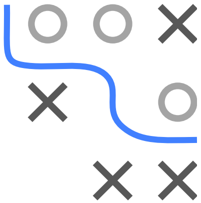




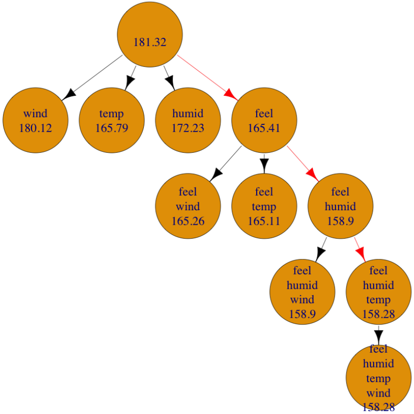
VISUALIZATION OF GFS

4. Iterate over this procedure



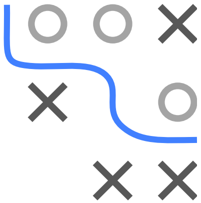


VISUALIZATION OF GFS



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

GREEDY BACKWARD SEARCH

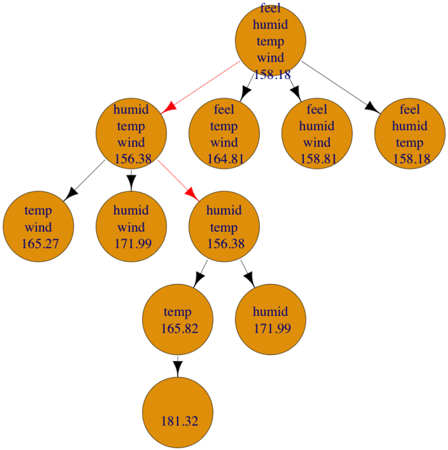


- Start with the full index set of features $S = \{1, \dots, p\}$.
- For a given set S generate all
  $S_j = S \setminus \{j\}$ with $j \in S$.
- Evaluate the classifier on all S_j and use the best S_j.
- Iterate over this procedure.
- Terminate if:
  - the performance drops drastically, or
  - falls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

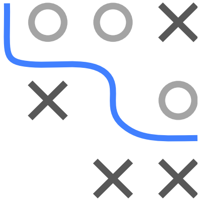
- GFS is much faster and generates sparser feature selections
- GBS much more costly and slower, but sometimes slightly better.

VISUALIZATION OF GBS

Example Greedy Backward Search on bike sharing data



EXTENSIONS

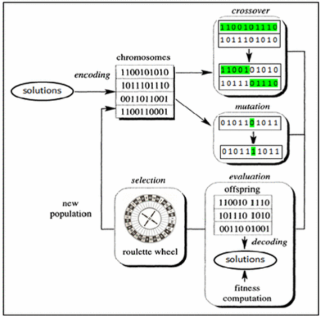


- Eliminate or add multiple features at once to increase speed
- Allow alternating forward and backward search (also known as stepwise model selection by AIC/BIC in statistics)
- Randomly sample candidate feature subsets in each iteration
- Focus search on regions of feature subsets where an improvement is more likely

EXTENSIONS: GENETIC ALGORITHMS FOR FS

Example Template for $(\mu + \lambda)$-Evolutionary Strategy applied to FS

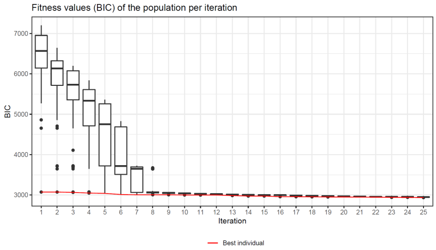
1. Initialization: μ random bit vectors (feature inclusion/exclusion)
2. Evaluate model performance for bit vectors
3. Select μ fittest bit vectors (parents)
4. Generate λ offspring applying crossover and mutation
5. Select μ fittest bit vectors from $(\mu + \lambda)$ options for next generation
6. Repeat steps 2-5 until stopping criterion is met

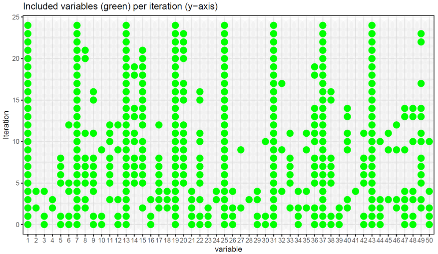


- Use CV/validation set for evaluation to avoid overfitting
- Choice of μ and λ allows some control over exploration vs. exploitation trade-off
- See our ▸ slds-lmu 2021 for further information

▸ Mitsuo Gen 1996

EXTENSIONS: GENETIC ALGORITHMS FOR FS

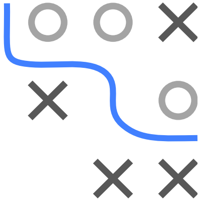




Top: BIC over number of iterations.

Bottom: Bit representation of selected features over iterations.

WRAPPERS



Advantages:

- Can be combined with any learner
- Any performance measure can be used
- Optimizes the desired criterion directly

Disadvantages:

- Evaluating target function is expensive
- Does not scale well with number of features
- Does not use additional info about model structure
- Nested resampling becomes necessary