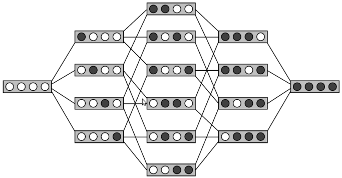
Introduction to Machine Learning

Feature Selection

Feature Selection: Wrapper methods



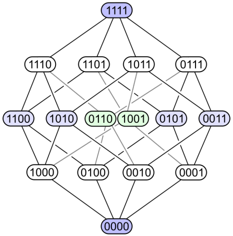
Learning goals

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

INTRODUCTION

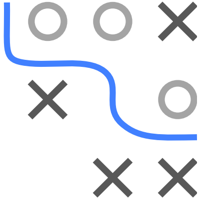
- Wrapper methods emerge from the idea that different sets of features can be optimal for different learners
- Wrapper is a discrete search strategy for S, where objective criterion is test error of learner as function of S. Criterion can also be calculated on train set, approximating test error (AIC, 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 $\Psi : \Omega \to \mathbb{R}$:

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

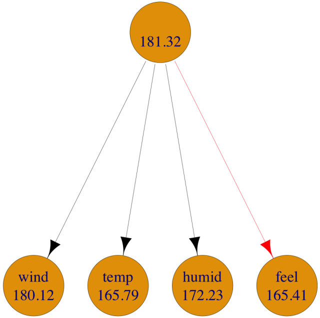
- Ω = search space of all feature subsets $S \subseteq \{1, \dots, p\}$. Usually we encode this by bit vectors, i.e., $\Omega = \{0, 1\}^p$ (1 = feat. selected)
- Objective Ψ can be different functions, e.g., AIC/BIC for LM or cross-validated performance of a learner
- Poses a discrete combinatorial 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 $S \subset \{1, \dots, p\}$ be subset of feature indices.

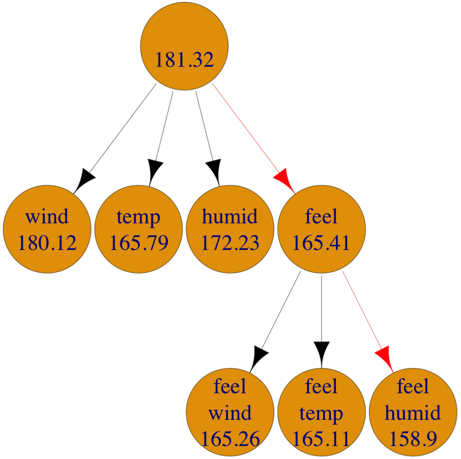
1. Start with the empty feature set $S = \emptyset$
2. For a given set S, generate all $S_j = S \cup \{j\}$ with $j \notin S$.
3. Evaluate the classifier on all S_j and use the best S_j

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



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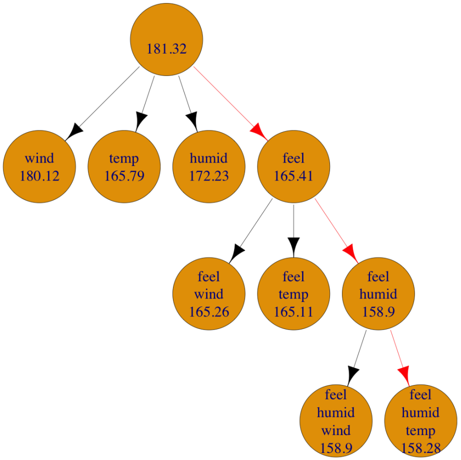
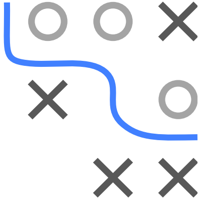
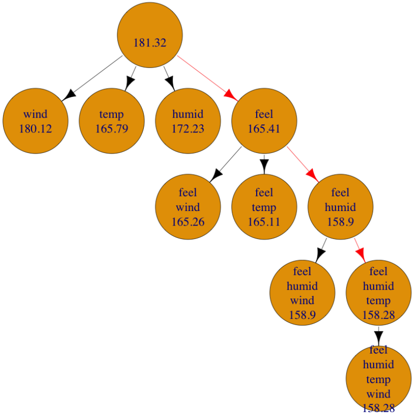
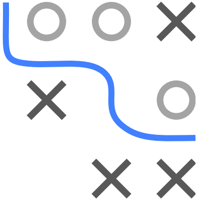




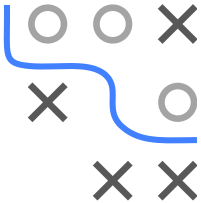
VISUALIZATION OF GFS





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

GREEDY BACKWARD SEARCH

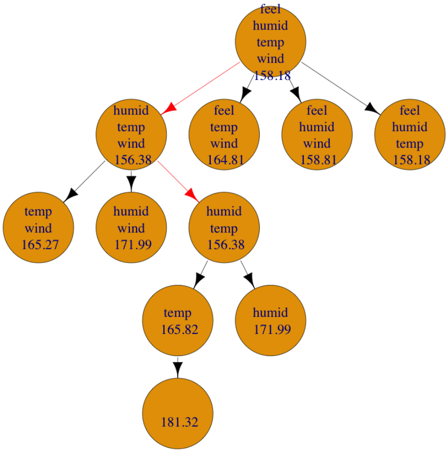


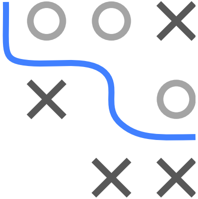
- Start with the full index set of features $S = \{1, \dots, p\}$.
- For a given set S generate all $S_j = S \setminus \{j\}$ with $j \in S$.
- Evaluate the classifier on all S_j and use the best S_j.
- Iterate over this procedure.
- Terminate if:
  - the performance drops drastically, or
  - falls below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

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

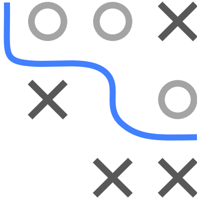
VISUALIZATION OF GBS

Example Greedy Backward Search on bike sharing data





EXTENSIONS

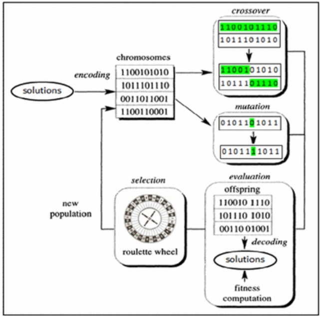


- Eliminate or add multiple features at once to increase speed
- Allow alternating forward and backward search (also known as stepwise model selection by AIC/BIC in statistics)
- Randomly sample candidate feature subsets in each iteration
- Focus search on regions of feature subsets where an improvement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

EXTENSIONS: GENETIC ALGORITHMS FOR FS

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

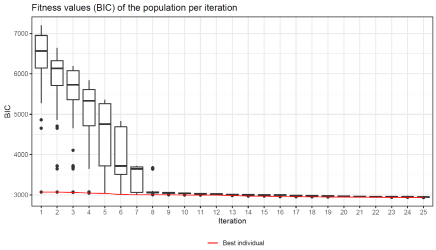
1. Initialization: μ random bit vectors (feature inclusion/exclusion)
2. Evaluate model performance for bit vectors
3. Select μ fittest bit vectors (parents)
4. Generate λ offspring applying crossover and mutation
5. Select μ fittest bit vectors from $(\mu + \lambda)$ options for next generation
6. Repeat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

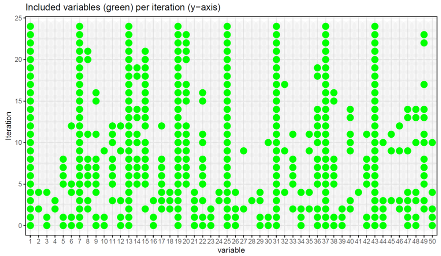


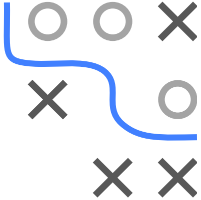
- Use CV/validation set for evaluation to avoid overfitting
- Choice of μ and λ allows some control over exploration vs. exploitation trade-off
- See our ▸ slds-lmu 2021 for further information

▸ Mitsuo Gen 1996

EXTENSIONS: GENETIC ALGORITHMS FOR FS



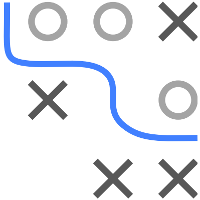




Top: BIC over number of iterations.

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