L12: randomized feature selection

Exponential search methods

- Branch and Bound
- Approximate monotonicity with Branch and Bound
- Beam Search

Randomized algorithms

- Random generation plus sequential selection
- Simulated annealing
- Genetic algorithms

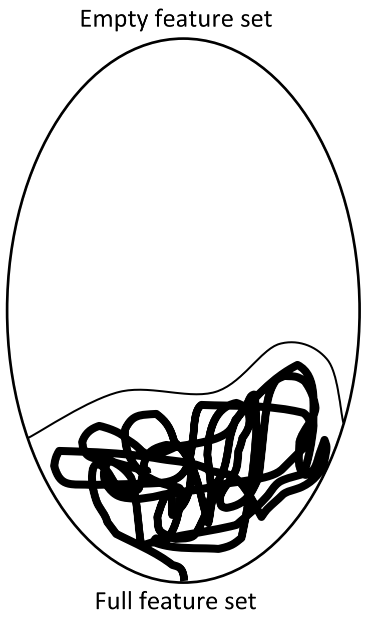
Branch and Bound (B&B)

Properties

- B&B [Narendra and Fukunaga, 1977] is guaranteed to find the optimal feature subset under the monotonicity assumption
  - The monotonicity assumption states that the addition of features can only increase the value of the objective function, that is

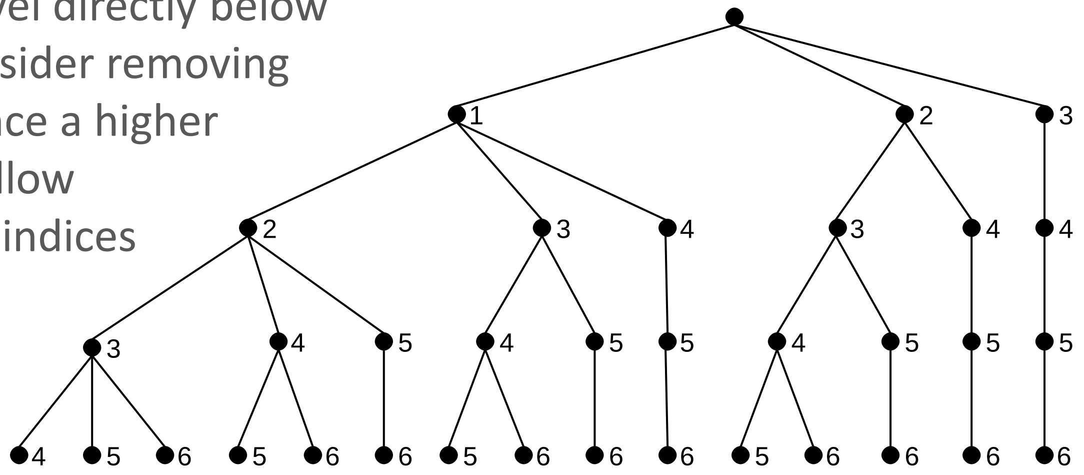
$$J(x_{i_1}) < J(x_{i_1}, x_{i_2}) < J(x_{i_1}, x_{i_2}, x_{i_3}) < \cdots$$

- Branch and Bound starts from the full set and removes features using a depth-first strategy
  - Nodes whose objective function are lower than the current best are not explored since the monotonicity assumption ensures that their children will not contain a better solution



Algorithm [Fukunaga, 1990]

- The algorithm is better explained by considering the subsets of $M' = N - M$ features already discarded, where N is the problem dimensionality and M is the desired number of features
- Since the order of the features is irrelevant, we will only consider an increasing ordering $i_1 < i_2 < \cdots i_M$, of the feature indices, this will avoid exploring states that differ only in the ordering of their features
- The Branch and Bound tree for $N = 6$ and $M = 2$ is shown below (numbers indicate features that are being removed)
  - Notice that at the level directly below the root we only consider removing features 1, 2 or 3, since a higher number would not allow sequences with four indices

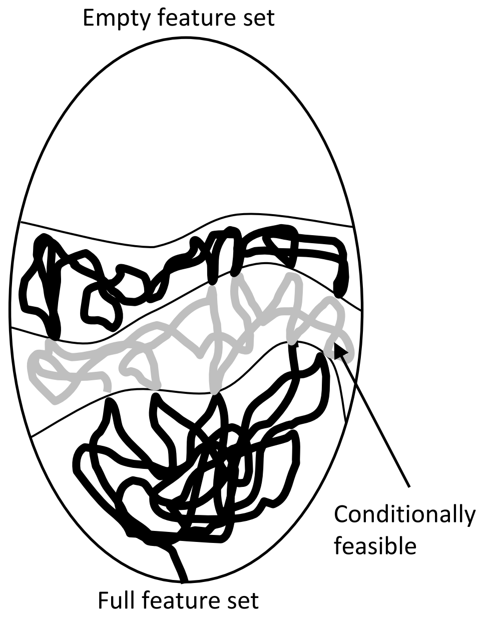


```
1. Initialize $\alpha = -\infty, k = 1$
2. Generate successors of the current node and store them in $LIST(k)$
3. Select new node
    if $LIST(k)$ is empty
        go to 5
    else
        $i_k = \underset{j \in LIST(k)}{\arg\max} J\left(x_{i_1}, x_{i_2} \dots x_{i_{k-1}}, j\right)$
        delete $i_k$ from $LIST(k)$
4. Check bound
    if $J\left(x_{i_1}, x_{i_2} \dots x_{i_k}\right) < \alpha$
        go to 5
    else if $k = M'$ (we have the desired number of features)
        go to 6
    else
        $k = k + 1$
        go to 2
5. Backtrack to lower level
        $k = k - 1$
        if $k = 0$
            terminate algorithm
        else
            go to 3
6. Last level
        Set $\alpha = J\left(x_{i_1}, x_{i_2} \dots x_{i_{k-1}}, j\right)$ and $Y_{M'}^{*} = \left\{x_{i_1}, x_{i_2} \dots x_{i_k}\right\}$
        go to 5
```

Approximate monotonicity B&B (AMB&B)

A variation of the classical B&B algorithm

- AMB&B allows non-monotonic functions to be used, typically classifiers, by relaxing the cutoff that terminates the search on a specific node
- Assume that we run B&B by setting a threshold error rate $E(Y) = \tau$ rather than a number of features M
- Under AMB&B, a given feature subset Y will be considered
  - **Feasible** if $E(Y) \leq \tau$
  - **Conditionally feasible** if $E(Y) \leq \tau\,(1 + \Delta)$
  - **Unfeasible** if $E(Y) \geq \tau\,(1 + \Delta)$
- where Δ is a tolerance placed on the threshold to accommodate for non-monotonic functions
- Rather than limiting the search to feasible nodes (as B&B does), AMB&B allows the search to explore conditionally feasible nodes in hopes that these will lead to a feasible solution
- However, AMB&B will not return conditionally feasible nodes as solutions, it only allows the search to go through them!
  - Otherwise it would not be any different than B&B with threshold $\tau\,(1 + \Delta)$



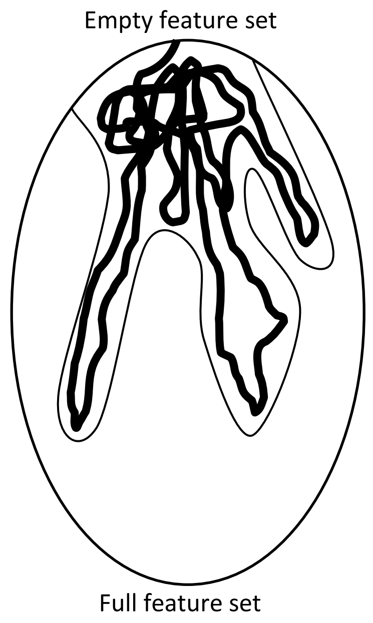
Beam search

Beam Search is a variation of best-first search with a bounded queue to limit the scope of the search

– The queue organizes states from best to worst, with the best states placed at the head of the queue

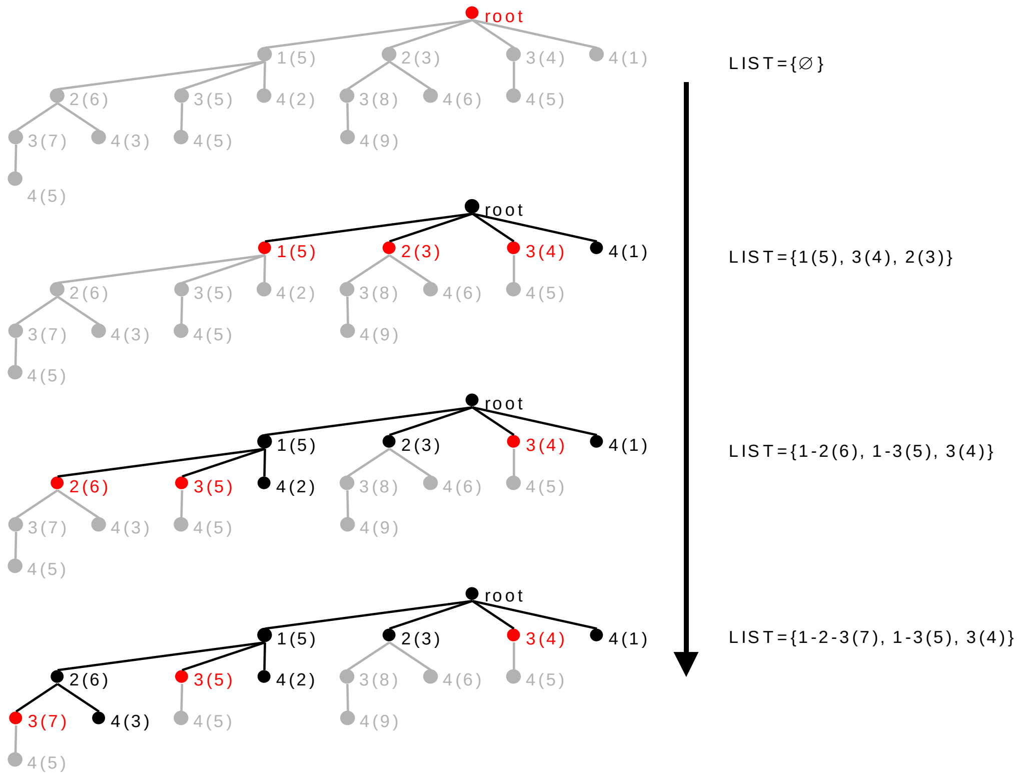
– At every iteration, BS evaluates all possible states that result from adding a feature to the feature subset, and the results are inserted into the queue in their proper locations

– Notice that BS degenerates to exhaustive search if there is no limit on queue size Similarly, if the queue size is set to one, BS is equivalent to SFS



Example: Run BS on a 4D search space and queue size = 3

– BS cannot guarantee that the optimal subset is found:
  - In the example, the optimal is 2-3-4 ($J = 9$), which is never explored
  - However, with the proper queue size, BS can avoid getting trapped in local minimal by preserving solutions from varying regions in the search space

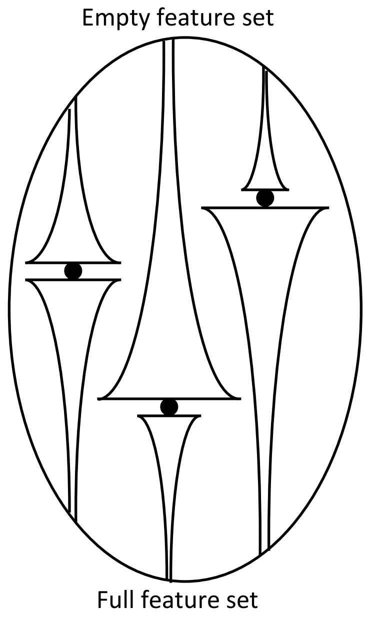


Random generation plus sequential selection

Approach

- An attempt to introduce randomness into SFS and SBS in order to escape local minima
- The algorithm is self-explanatory

```
1. Repeat for a number of iterations
    - Generate a random feature subset
    - Perform SFS on the subset
    - Perform SBS on the subset
```



Simulated annealing

A stochastic optimization method that derives its name from the annealing process used to re-crystallize metals

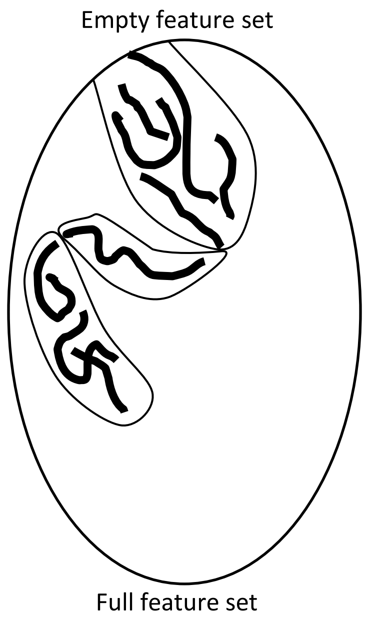
- During the annealing process in metals, the alloy is cooled down slowly to allow its atoms to reach a configuration of minimum energy (a perfectly regular crystal)
  - If the alloy is annealed too fast, such an organization cannot propagate throughout the material
  - The result will be a material with regions of regular structure separated by boundaries
  - These boundaries are potential fault-lines where fractures are most likely to occur when the material is stressed
- The laws of thermodynamics state that, at temperature T, the probability of an increase in energy ΔE in the system is given by the expression

$$P(\Delta E) = e^{-\frac{\Delta E}{kT}}$$

  - where k is known as Boltzmann's constant

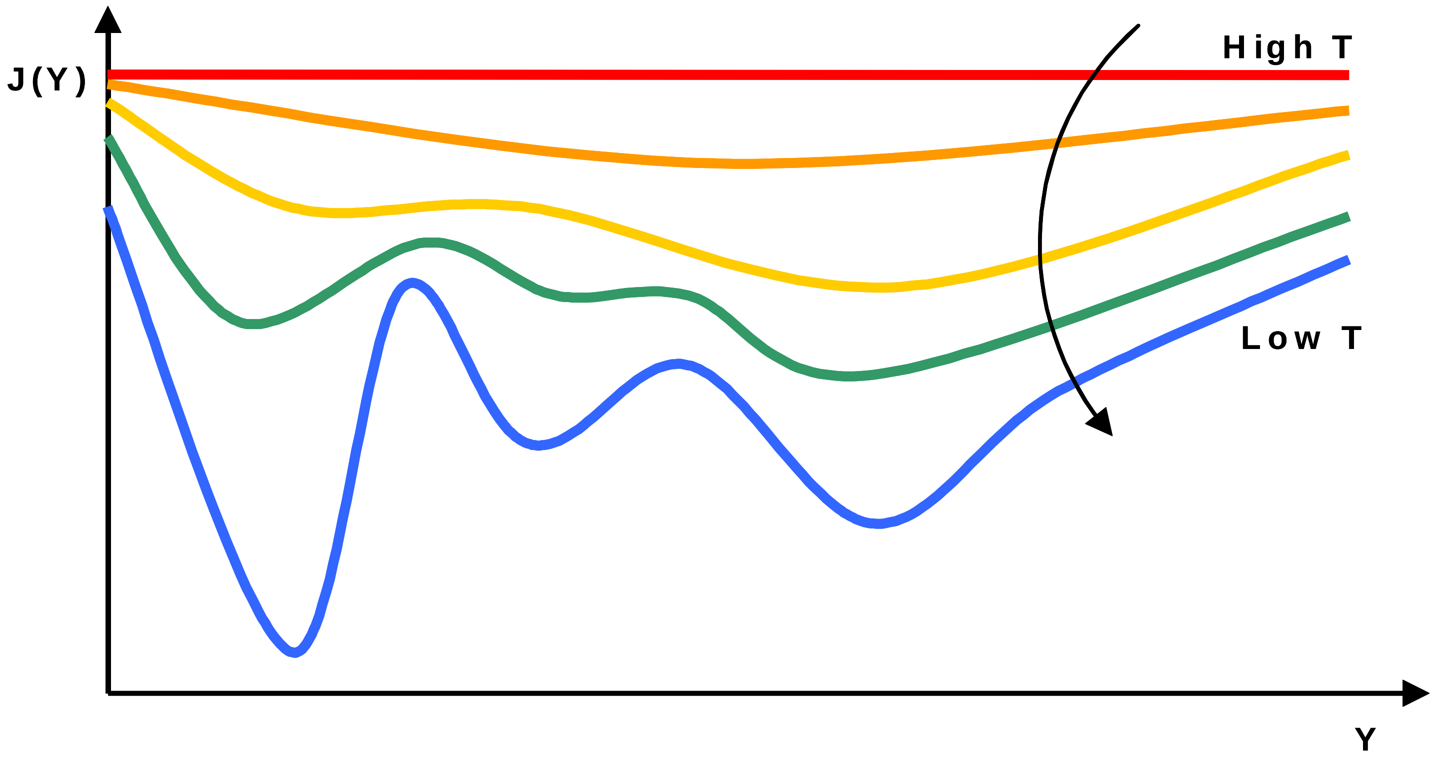
– SA is a straightforward implementation of these ideas

```
1. Determine an annealing schedule $T_i$
2. Create an initial solution $Y_0$
3. While $T_i > T_{MIN}$
    - Generate a new solution $Y_{i+1}$ as a local search on $Y_i$
    - Compute $\Delta E = J(Y_i - Y_{i+1})$
    - If $\Delta E < 0$
        then
            always accept the move from $Y_i$ to $Y_{i+1}$
        else
            accept the move with probability $P = e^{-\Delta E/(T_i)}$
```



- **SA is summarized with the following idea**
  - *"When optimizing a very large and complex system (i.e., a system with many degrees of freedom) , instead of always going downhill, try to go downhill most of the times"* [Haykin, 1999]
- **The previous formulation of SA can be used for any type of minimization problem and it only requires specification of**
  - A transform to generate a local neighbor from the current solution (i.e. add a random vector)
    - For FSS, the transform will consist of adding or removing features, typically implemented as a random mutation with low probability
  - An annealing schedule, typically $T_{i+1} = rT_i$, with $0 \leq r \leq 1$
  - An initial temperature T_0
- **Selection of the annealing schedule is critical**
  - If r is too large, the temperature decreases very slowly, allowing moves to higher energy states to occur more frequently; this slows convergence
  - If r is too small, the temperature decreases very fast, and the algorithm is likely to converge to a local minima

- A unique feature of simulated annealing is its adaptive nature
- At high temperature the algorithm is only looking at the gross features of the optimization surface, while at low temperatures, the finer details of the surface start to appear

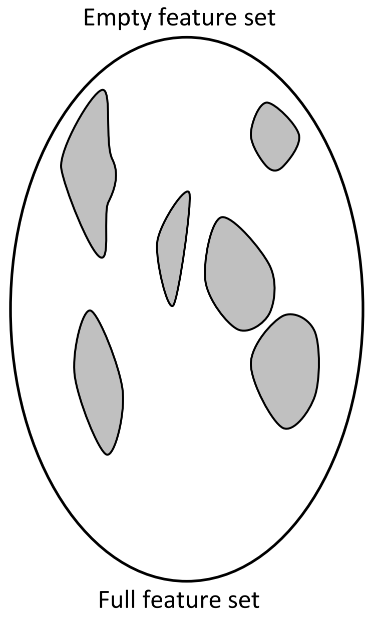


Genetic algorithms

GAs are an optimization technique inspired by evolution (survival of the fittest)

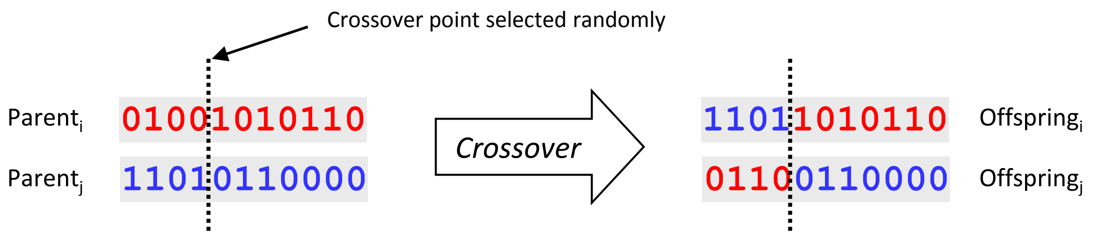
- Starting with an initial random population of solutions, evolve new populations by mating (crossover) pairs of solutions and mutating solutions according to their fitness (objective function)
- The better solutions are more likely to be selected for the mating and mutation operations and therefore carry their "genetic code" from generation to generation
  - For FSS, solutions are simply represented with an indicator variable [Holland in 1974]

```
1. Create an initial random population
2. Evaluate initial population
3. Repeat until convergence (or a number of generations)
   - Select the fittest individuals in the population
   - Create offsprings through crossover on selected individuals
   - Mutate selected individuals
   - Create new population from the old population and the offspring
   - Evaluate the new population
```



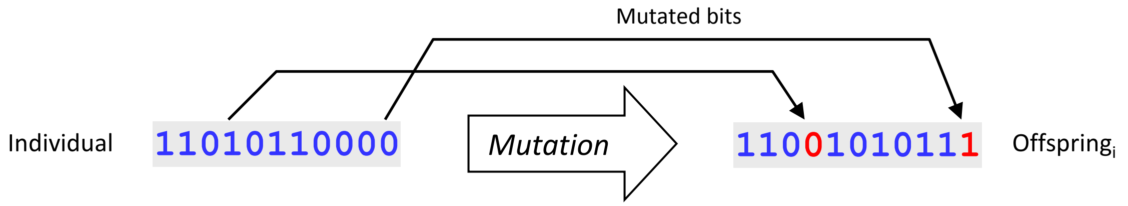
Single-point crossover

- Select two individuals (parents) according to their fitness
- Select a crossover point
- With probability P_C (0.95 is reasonable) create two offspring by combining the parents



Binary mutation

- Select an individual according to its fitness
- With probability P_M (0.01 is reasonable) mutate each one of its bits



Selection methods

The selection of individuals is based on their fitness value

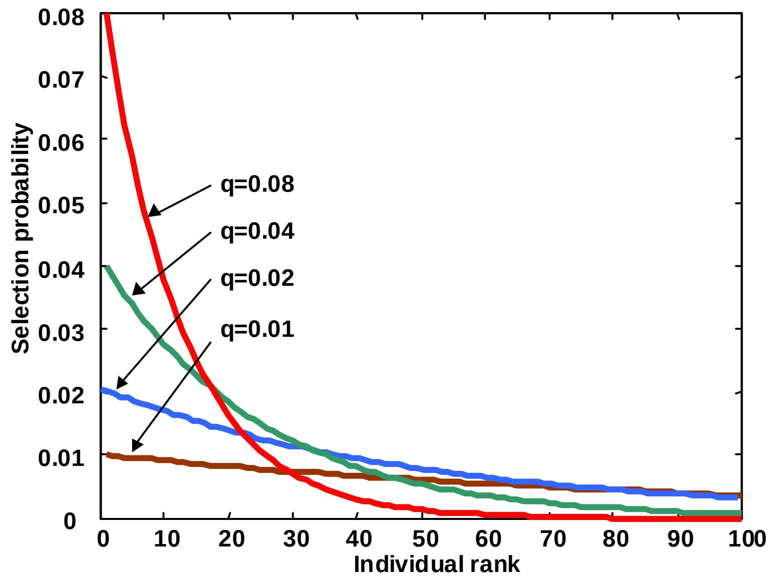
- We will describe a selection method called Geometric selection
- Other methods are available: Roulette Wheel, Tournament Selection …

Geometric selection

- The probability of selecting the r^{th} best individual is given by the geometric distribution

$$P(r) = q(1-q)^{r-1}$$

  - where q is the probability of selecting the best individual (0.05 being a reasonable value)



- Therefore, the geometric distribution assigns higher probability to individuals ranked better, but also allows unfit individuals to be selected
- In addition, it is typical to carry the best individual of each population to the next one; this is called the Elitist Model

GA parameter choices for FSS

The choice of crossover rate P_C is important

- You will want a value close to 1.0 to have a large number of offspring
- The optimal value is inversely proportional to population size [Doak, 1992]

The choice of mutation rate P_M is very critical

- An optimal choice will allow the GA to explore the more promising regions while avoiding getting trapped in local minima
  - A large value (i.e., $P_M > 0.25$) will not allow the search to focus on the better regions, and the GA will perform like random search
  - A small value (i.e., $P \approx 0$) will not allow the search to escape local minima

The choice of q, the probability of selecting the best individual, is also critical

- An optimal value of q will allow the GA to explore the most promising solution, and at the same time provide sufficient diversity to avoid early convergence of the algorithm

In general, poorly selected control parameters will result in sub-optimal solutions due to early convergence

Search strategies –summary

	Accuracy	Complexity	Advantages	Disadvantages
Exhaustive	Always finds the optimal solution	Exponential	High accuracy	High complexity
Sequential	Good if no backtracking needed	Quadratic $O(N_{EX}^2)$	Simple and fast	Cannot backtrack
Randomized	Good with proper control parameters	Generally low	Designed to escape local minima	Difficult to choose good parameters

– A highly recommended review of the material presented in these two lectures is

Justin Doak
"An evaluation of feature selection methods and their application to Computer Security"
University of California at Davis, Tech Report CSE-92-18