Genetic algorithm for variable selection

Jaakko Väyrynen
jaakko.j.vayrynen@tkk.fi

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References

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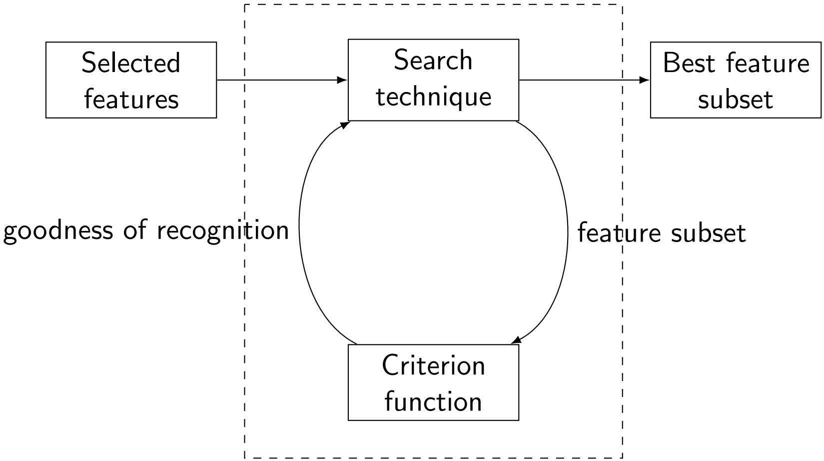
Feature selection techniques

- Tradeoff between accuracy and performance
- Search for "optimal" subset of features
- Problem specific heuristics (filter methods)
  - Domain knowledge is available
  - Prune search space based on domain knowledge
- General heuristics (wrapper methods)
  - Domain knowledge is unavailable or costly to exploit
  - Mainly hill-climbing algorithms

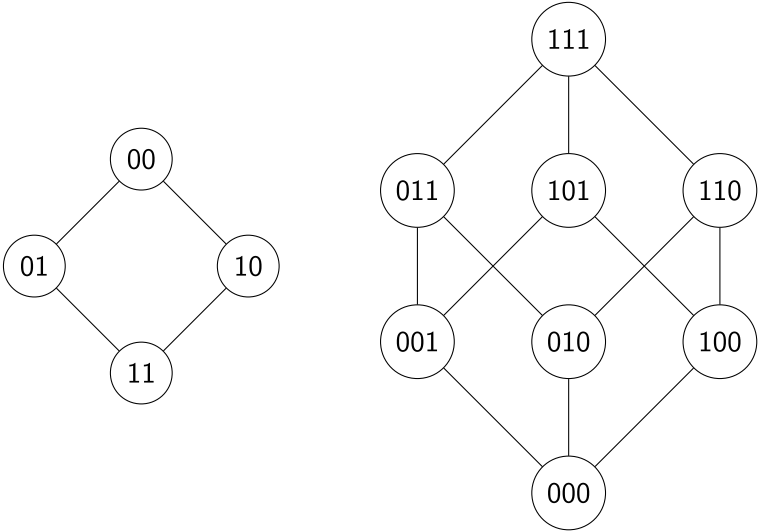
Feature selection process for wrapper approach



Sequential backward selection (SBS) algorithm

- Try removing each remaining feature one at a time
- Permanently remove the feature giving the least improvement
- Measure improvement with domain specific criterion function
- Greedy algorithm
  - Early mistakes cannot be canceled
  - Easily gets stuck at local optima
  - Does not consider effects of removing a set of features
- Running time $\mathcal{O}(n^2)$

Greedy feature selection lattice



Source of brittleness

- $f(x_0, x_1, x_2) = ax_0 + bx_1 + cx_2 + dx_0x_1 + ex_0x_2 + fx_1x_2 + gx_0x_1x_2$

Source of brittleness

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- With $b = c, d = e = 0$

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- With $b = c, d = e = 0$
- Value assignments to all feature subsets

x_0, x_1, x_2	$f(x_0, x_1, x_2)$	constraint
000	0	
100	a	(global optimum)
001	b	
010	b	
011	$2b + f$	(local optimum)
101	$a + b$	
110	$a + b$	
111	$a + 2b + f + g$	

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- Let $m = 2b + f$

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- Let $m = 2b + f$
- Global optimum implies that
  $a > 0, a > b, a > m, a > a + b, \dots$
  $a > 0 \wedge a > a + b \Rightarrow b < 0$

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110	$a + b$	
111	$a + m + g$	

- Let $m = 2b + f$, $b = -4, f = 9$
- Global optimum implies that
  $a > 0, a > b, a > m, a > a + b, \ldots$
  $a > 0 \land a > a + b \Rightarrow b < 0$
- Local optimum implies that $m > a + b$, $g < -a$

Source of brittleness

- $f(x_0, x_1, x_2) = ax_0 - 4x_1 - 4x_2 + 9x_1x_2 + gx_0x_1x_2$
- Value assignments to all feature subsets

x_0, x_1, x_2	$f(x_0, x_1, x_2)$	constraint
000	0	
100	a	(global optimum)
001	-4	
010	-4	
011	m	(local optimum)
101	$a-4$	
110	$a-4$	
111	$a+m+g$	

- Let $m = 1$, $b = -4, f = 9$
- Global optimum implies that
  $a > 0, a > b, a > m, a > a + b, \ldots$
  $a > 0 \wedge a > a + b \Rightarrow b < 0$
- Local optimum implies that $m > a + b$, $g < -a$

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- Global optimum implies that
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x_0, x_1, x_2	$f(x_0, x_1, x_2)$	constraint
000	0	
100	a	(global optimum)
001	-4	
010	-4	
011	1	(local optimum)
101	$a - 4$	
110	$a - 4$	
111	$a + 1 + g$	

- Let $m = 1$, $b = -4, f = 9$
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011	1	(local optimum)
101	$a-4$	
110	$a-4$	
111	$a+1+g$	

- Let $m = 1$, $b = -4, f = 9$, $g = -5$
- Global optimum implies that
  $a > 0, a > b, a > m, a > a + b, \ldots$
  $a > 0 \wedge a > a + b \Rightarrow b < 0$
- Local optimum implies that $m > a + b$, $g < -a$

Source of brittleness

- $f(x_0, x_1, x_2) = ax_0 - 4x_1 - 4x_2 + 9x_1x_2 - 5x_0x_1x_2$
- Value assignments to all feature subsets

x_0, x_1, x_2	$f(x_0, x_1, x_2)$	constraint
000	0	
100	a	(global optimum)
001	-4	
010	-4	
011	1	(local optimum)
101	$a - 4$	
110	$a - 4$	
111	$a + 1 - 5$	

- Let $m = 1$, $b = -4, f = 9$, $g = -5$
- Global optimum implies that
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  $a > 0 \wedge a > a + b \Rightarrow b < 0$
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111	$a-4$	

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- Global optimum implies that
  $a > 0, a > b, a > m, a > a + b, \ldots$
  $a > 0 \wedge a > a + b \Rightarrow b < 0$
- Local optimum implies that $m > a + b$, $g < -a$
- Constraints apply when $1 < a < 5$

Genetic algorithm (GA)

- Motivation from genetics
- Representations for solutions (chromosomes)
- Maintains a number of solutions (population)
- Performs search in the space of solutions (evolution)
  - Combines solutions (chromosome mixing)
  - Inserts/modifies random properties (mutation)
  - Better solutions reproduce more likely ("survival of the fittest")
- Does not require continuity etc.
- Has been shown to find good solutions to hard problems
- No proof of convergence
- Is usually slow
- Heuristic implementation for each problem

Basic genetic algorithm

1. Initial population P_0 of N individuals with fitness values
2. $G \leftarrow 1$
3. $P'_G \leftarrow selection\_function(P_G - 1)$
4. $P_G \leftarrow reproduction\_function(P'_G)$
5. $F_G \leftarrow evaluate\_fitness(P_G)$
6. $G \leftarrow G + 1$
7. Repeat step 3 until termination
8. Print out best solution found

- How to represent solutions?
- How to initialize?
- How to evaluate fitness of each individual?
- How to select individuals for reproduction?
- How to accomplish reproduction?
- When to terminate?

Solution representation

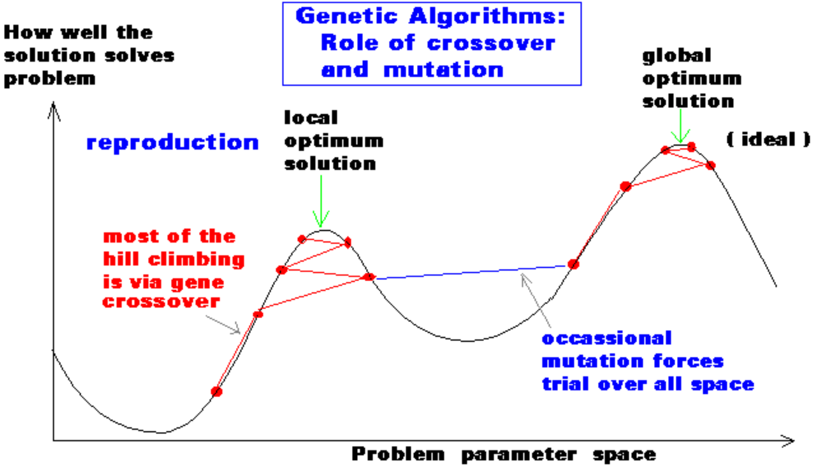
- Structure of the solution
- Linked to reproduction (genetic operations)
- An individual is represented by (a sequence of) genes from an alphabet
- Alphabet: binary, (bounded) floats, integers, sets, symbols, matrices, graphs, model parameters, etc.

Selection function

- Defines which individuals produce next generations
- Good individuals have better chance to get selected
- Techniques: roulette wheel, scaling techniques, tournament, elitist models, ranking models
- Probability P_i for the selection of i:th individual
  - Roulette wheel $P_i = \frac{F_i}{\sum_j F_j}$, with fitness F_i
  - Windowing and scaling allows minimization and negativity
  - Normalized ranking $P_i = q'(1-q)^{r-1}$
    - $q =$ probability of selecting the best individual
    - $r =$ the rank of the individual, where 1 is the best
    - $N =$ the population size
    - $q' = \frac{q}{1-(1-q)^N}$
- Tournament selection
  - Select j items randomly (with replacement)
  - Insert the best of j into the new population
  - Repeat until N individuals have been selected

Genetic operators

- Search mechanism in GA
- Creates new solutions based on existing solutions
- Implementation depends on chromosome representation
- Crossover takes two solutions and produces two new solutions
- Mutation takes one solution and produces one new solution



from http://www.sussex.ac.uk/space-science/ga.html

Crossover and mutation for binary valued vectors

- Let $\bar{X} = (x_1, ..., x_m)$ and $\bar{Y} = (y_1, ..., y_m)$ be two selected m-dimensional binary-valued row vectors
- Mutation flips each bit with probability p_m:
$$x_i' = \begin{cases} 1 - x_i, & \text{if } U(0,1) < p_m \\ x_i, & \text{otherwise} \end{cases}$$
- Inversion is mutation with probability $p_m = 1$
- Crossover splits and joins the parents from bit $r = U(1, m)$:
$$x_i' = \begin{cases} x_i, & \text{if } i < r \\ y_i, & \text{otherwise} \end{cases} \text{ and } y_i' = \begin{cases} y_i, & \text{if } i < r \\ x_i, & \text{otherwise} \end{cases}$$
- Variations: single split, multiple splits, different splits

Crossover and mutation for bounded floats

- Let $\bar{X}$ and $\bar{Y}$ be two selected m-dimensional float-valued row vectors with lower bound a_i and upper bound b_i for each variable, and j is a randomly selected variable, $r = U(0, 1)$
- Arithmetic crossover: $\begin{array}{l} \bar{X}' = r\bar{X} + (1-r)\bar{Y} \\ \bar{Y}' = (1-r)\bar{X} + r\bar{Y} \end{array}$
- Heuristic crossover, with $F(\bar{X}) > F(\bar{Y})$: $\begin{array}{l} \bar{X}' = \bar{X} + r(\bar{X} - \bar{Y}) \\ \bar{Y}' = \bar{X} \end{array}$

  if $x_i' \geq a_i, x_i' \leq b_i \quad \forall i$, otherwise recalculate at most t times
- Uniform mutation: $x_i' = \begin{cases} U(a_i, b_i), & \text{if } i = j \\ x_i, & \text{otherwise} \end{cases}$

- Boundary mutation changes value to its upper or lower bound:

$$x_i' = \begin{cases} a_i, & \text{if } i = j, r < 0.5 \\ b_i, & \text{if } i = j, r \geq 0.5 \\ x_i, & \text{otherwise} \end{cases}$$

- Non-uniform mutation:

$$x_i' = \begin{cases} x_i + (b_i - x_i)f(G), & \text{if } i = j, r_1 < 0.5 \\ x_i - (x_i + a_i)f(G), & \text{if } i = j, r_1 \geq 0.5 \\ x_i, & \text{otherwise} \end{cases}$$

$$f(G) = (r_2(1 - \frac{G}{G_{max}}))^b$$

where

$$\begin{aligned} r_k &= U(0,1),\ k \in \{0,1\} \\ G &= \text{the current generation number} \\ G_{max} &= \text{the maximum number of generations} \\ b &= \text{a shape parameter} \end{aligned}$$

- Multi-non-uniform mutation

Initialization, termination and evaluation

- Selection of initial population P_0
  - Random solutions from the search space
  - Approximate solutions found with other methods
  - Solutions from experts
  - Mixtures of these
- Termination criterion
  - Maximum number of generations G_{max}
  - Population convergence criteria
  - Lack of improvement within a number of generations
  - External evaluation measure
- Fitness evaluation functions
  - Minimal requirement: map the population into a partially ordered set

Genetic algorithm for variable selection

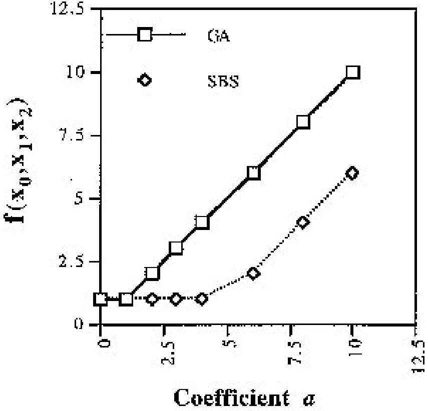
- Representation: Binary string where 1 is for selected and 0 for unselect variable
- Initialization: Random
- Evaluation: Cost function with selected variables
- Selection: Any binary selection method
- Genetic operators: Binary mutation and crossover (and inversion)
- Termination: Any

Compare SBS and GA with toy data

- $f(x_0, x_1, x_2) = ax_0 - 4x_1 - 4x_2 + 9x_1x_2 - 5x_0x_1x_2$
- If $0 < a < 1$, 011 is the global optimum
- If $a > 1$, global optimum is 100 with value a
- If $1 < a < 5$, 011 is the local optimum
- If $a \geq 5$, 111 is a local optimum
- GENESIS program was used with parameters
  - Population size 50
  - Crossover rate 0.6
  - Mutation rate 0.001 for the new generation

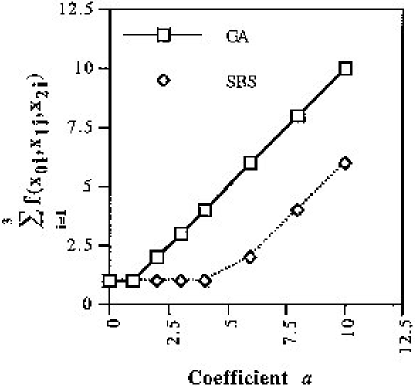
Toy data: add undepended features

- Add additional 27 features to create search space of 2^{30}
- Vary a



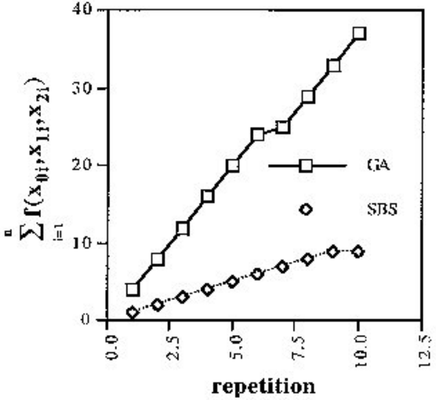
Toy data: replicate depended features

- Replicate depended features 3 times
- Add additional 21 features to create search space of 2^{30}
- Vary a



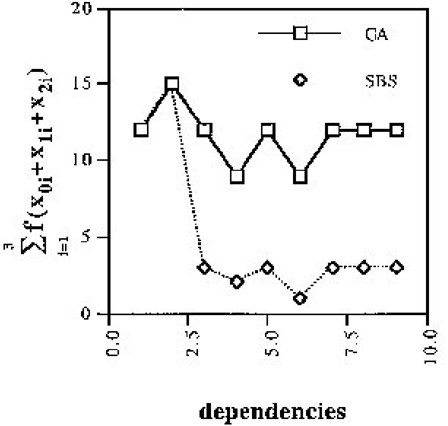
Toy data: number or replications

- Let $a = 4$
- Vary number of replications n of depended features
- Add additional features to create search space of 2^{30}



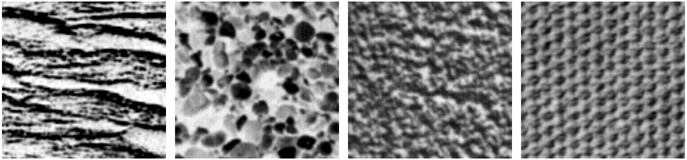
Toy data: number or dependencies

- Let $a = 4$
- Vary number of m-feature dependencies by overlapping 3-feature dependencies

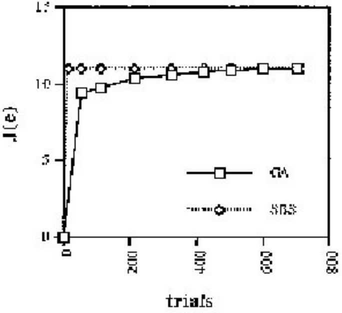


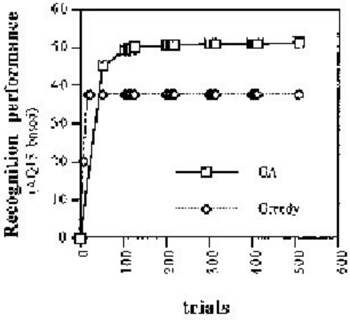
Compare SBS and GA with texture classification task

- Four textures from Brodatz album of textures
- 18 features
- 100 samples of size 30×30 pixels from each image
- Goal: optimal feature set for AQ15 for inducing texture classification rules
- Two evaluation functions
  - Heuristic evaluation function as the maximal separation of classes
  - Exact evaluation by first training AQ15 and testing classification accuracy on test data



Texture classification experiment results





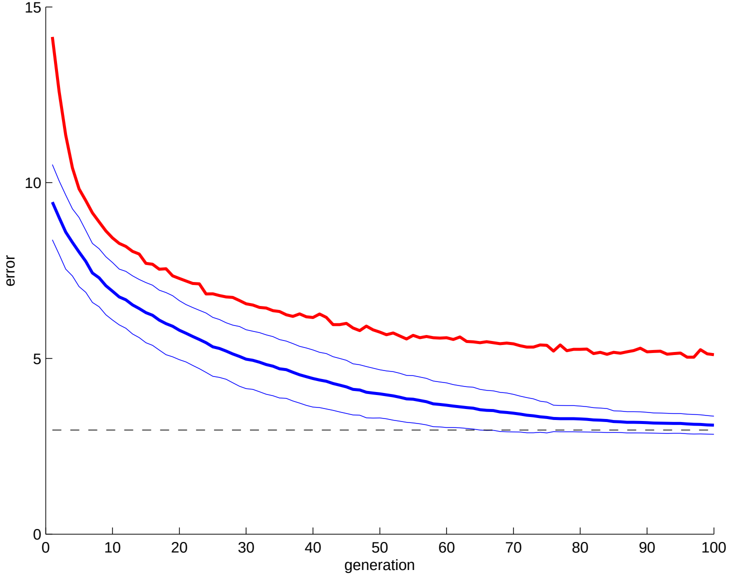
Implementation of GA for variable selection

- Implemented in Matlab with
  - Binary representation
  - Different cost (fitness) functions
  - Roulette wheel selection
  - Survival of the elite
  - Reproduction: binary mutation and crossover
  - Termination after N generations
- Problems
  - Slow with KNN and lots of samples and large population

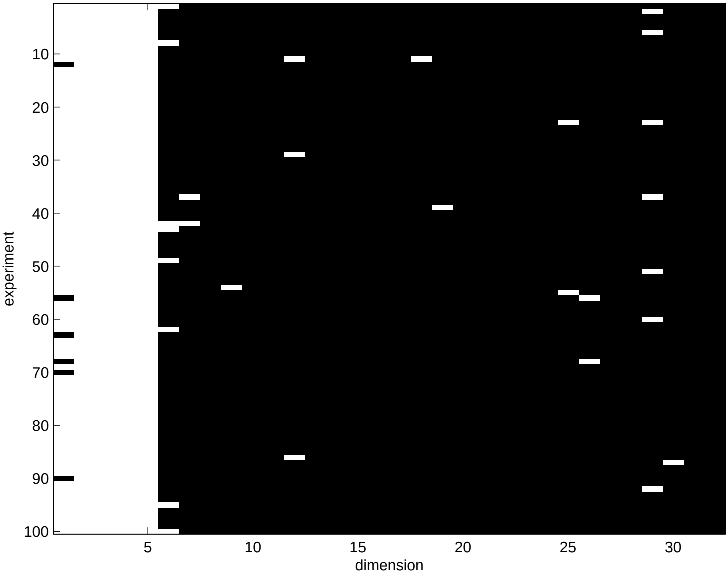
Experiment with implementation

- $y = x_1 - 2x_2 - 3x_3 + 2x_4x_5 + 0.1z$
  $x_6 = x_1x_2$
  $x_7 = x_2x_9$
  $x_8 = x_3x_{10}$
  $z, x_i \sim \mathcal{N}(0,1),\ i \in [1,32]$
- 300 samples, $2^{32} \approx 10^9$ input combinations
- Population size 10 of which 2 was elite
- Random initialization with equal chances for each bit
- KNN cost function
- Roulette wheel selection proportional to costs
- Reproduction functions with equal chance
  - Crossover with equal chance
  - Mutation with 0.1 chance for flip for each bit
- Termination after 100 generations

Best solution and average population development



Best individuals for the experiments



Summary

- Genetic algorithms are very heuristic
- They can find good solutions to hard problems
- Can do variable selection