Linear and Combinatorial Optimizations by Estimation of Distribution Algorithms

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January 17, 2003
9th MPS Symposium, Japan

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Genetic Algorithms

• Genetic Algorithms are popular because
  - Easy to use
  - Can be applied without prior knowledge
  - Parallelization can used
• Problems in Genetic Algorithms
  - Complex interactions among variables
  - Sometimes very difficult to get solutions

Estimation of Distribution Algorithm (EDA)

• Use probabilistic models for recombination
• Learn and sample that probabilistic models to generate new solutions
• Selection and replacement strategy of GA can be used
• Allow adaptation and improve expressiveness
Other Names of EDAs

- Probabilistic Model Building Genetic Algorithms (PMBGAs)
- Distribution Estimation Algorithms (DEAs)
- Iterated Density Estimation Algorithms (IDEAs)

Pseudocode of EDA

1. Generate initial population
2. Select some promising individuals
3. Build probabilistic model using selected individuals
4. Sample the model to generate new individuals
5. Replace old population by new individuals
6. If Termination_Criteria not satisfied go to 2

Discrete EDAs

- **Univariate**: no dependency among variables
  
  Example: UMDA, PBIL, CGA

- **Bivariate**: pairwise dependency
  
  Example: MIMIC, COMIT, BMDA

- **Multivariate**: multiple dependencies
  
  Example: BOA, EBNA, ECGA, FDA, LFDA

Univariate EDAs

- **Univariate Marginal Distribution Algorithm (UMDA)** (Mühlenbein et.al, 1996)
- **Population Based Incremental Learning (PBIL)** (Baluja, 1994)
- **Compact Genetic Algorithm (CGA)** (Harik et.al, 1998)

  - PBIL and CGA use probability vector \( p \) while UMDA uses population
  
  - PBIL and CGA use different update rules for \( p \)
UMDA

- Uses a probability vector $p=(p_1, p_2, \ldots, p_n)$
  - $p_i$ is the probability of 1 in the $i$th position
- Compute $p$ from selected individuals
- Generate 1 in the position $i$ with prob. $p_i$
- Approximates the behavior of uniform crossover of GA
- Problem: Joint probability may be 0 due to some $p_i=0$ and may converge to local optimal

Laplace Correction for UMDA

- Now joint probability distribution $>0$
- Marginal probability of each variable $X_i$ is calculated as
  $$p(x_i \mid D_i^{(n)}) = \frac{\sum_{j=1}^{N} \delta_j (X_i = x_i \mid D_i^{(n)}) + 1}{N + r_i}$$
  - $r_i$ is the number of different values $X_i$ may take

Bivariate EDAs

- Mutual Information Maximization for Input Clustering (MIMIC) (De Bonet et al., 1997)
- Combining Optimizers with Mutual Information Trees (COMIT) (Baluja et al., 1997)
- Bivariate Marginal Distribution Algorithm (BMDA) (Pelikan et al. 1999)
- They learn two order structures and are easy to use
**Multivariate EDAs**

- Extended Compact Genetic Algorithm (ECGA) (Harik 1999)
- Bayesian Optimization Algorithm (BOA) (Pelikan et al., 2000)
- Estimation of Bayesian Networks Algorithm (EBNA) (Etxeberria et al., 1999)
- Factorized Distribution Algorithm (FDA) (Mühlenbein et al., 1999)
- Learning Factorized Distribution Algorithm (LFDA) (Mühlenbein et al., 1999)

**BOA, EBNA and LFDA**

- Uses Bayesian Network but different score metrics:
  - **BOA**: Bayesian Dirichlet Equivalence (BDe) metric
  - **EBNA**: BIC, K2+Penalization scores
  - **LFDA**: BIC but restriction on no. of parents

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**Structure Learning in Bayesian Network**

1. Start with empty graph (no edges)
2. Apply primitive graph operators
3. Pick the operation that increases score
4. Perform that operation
5. If no improvement or constraints violates, stop else go to 2.

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**FDA**

- Applicable to *Additively Decomposable Problem*
- Uses *Boltzmann Selection* and calculate Boltzmann distribution
- Needs *structure learning* as well as parameters learning
ECGA

- Uses Greedy Search and BIC score
- For Search
  - Start with one bit group
  - Merge two groups if improves
  - No more improvement, finish

Summary of Multivariate EDAs

- Bayesian Network is mostly used
- But learning model structure is very difficult (NP hard)
- Can successfully solve problems decomposable into sub problems of bounded difficulty

Different Problems Considered

1. OneMax
2. Subset Sum
3. N-Queen
   - Algorithm used: UMDA with Laplace correction
   - Selection( for UMDA): Truncation Selection (best half of the population)
   - Replacement: Elitism

OneMax Function

- Return sum of the bits
- Optimum: All 1s \(\{1,1,\ldots,1\}\)
- Fitness: sum of variables in an individual
- Terminate: when fitness=problem size
- GA: One point crossover and mutation
Subset Sum Problem

- **Definition:** What subset of a set of integers has the sum equal to expected weight
- **Example:** Given \( l = \{1, 3, 5, 6, 8, 10\} \), \( W = 14 \)
  - **Solution:** \( \{1, 3, 10\}, \{3, 5, 6\}, \{6, 8\}, \{1, 5, 8\} \)
- **Trivial case:** Sum of all integers = Weight
- **Random case:** Sum of all integers > Weight

UMDA and GA for Subset Sum Problem

- **Fitness:** Absolute difference between sum of variables in an individual and expected weight
- **Termination:** Sum of variables in an individual equal to expected weight
- **GA:** one point crossover and mutation

n-Queen Problem

- **Definition:** place \( n \) queens on a \( n \times n \) chessboard so that no two queens attack each other i.e. they are not on the same row, column or diagonal
- **How?** If \( \text{abs(row}_i - \text{row}_j) = \text{abs(column}_i - \text{column}_j) \)
- **Example:** 4-Queen solutions

Solution of n-Queen Problem

- **Solution Encoded:** \( \{X_1, X_2, ..., X_n\} \)
  - \( X_i \) indicates the column position of \( i \)th queen at row \( i \)
- **Probability Vector:** 2-dimensional
  - Each \( p_{ij} \) indicates the probability of variable \( X_j \) taking its \( j \)th value at position \( i \)
- **Fitness:** no. of queens at non-attacking positions
GA for n-Queen Problem

- **Crossover**: Partially Matched Crossover (PMX)
- **Mutation**: Greedy Swap Mutation
- **Termination**: When all the queens are at non-attacking positions
- Very efficient than UMDA

Local Heuristics for n-Queen

- To improve performance of UMDA 2-opt algorithm as local heuristic used
- But GA with PMX still better

Probabilistic Modification for n-Queen

- When a variable is selected for a position, its probability for other positions must be zero
- If Roulette Wheel selection is used probabilistic modification ensure distinct values for different positions

Experimental Results (Subset Sum Problem)-I

- Average no. of generations required
- Average Time(sec) required

Average no. of generations and time(sec) for trivial solution
Experimental Results
(Subset Sum Problem)-II

Average generations required

No. of generations
Problem Size

0 5 10 15 20 25 30

0 20 40 60 80 100

Experimental Results
(OneMax Function)

Average Time(sec) required

No. of generations
Problem Size

0 0.2 0.4 0.6 0.8 1

0 50 100

Experimental Results
(n-Queen Problem)

Average Time(sec) Required for n-Queen problem

No. of Queens

0 20 40

0 20 40 60 80 100

Summary

• UMDA better than GA for some linear problems of independent variables
• To Capture higher order dependency we have to consider BOA, ECGA, FDA or EBNA
• BOA and EBNA may be general approach for a problem
Future Works

- Understand the behavior of BOA, EBNA, FDA etc.
- Apply EDA to permutation domains
- Develop an EDA for discrete and continuous domain