

# Probabilistic Model-Building Genetic Algorithms

a.k.a. Estimation of Distribution Algorithms  
a.k.a. Iterated Density Estimation Algorithms

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## Foreword

- Motivation
  - Genetic and evolutionary computation (GEC) popular.
  - Toy problems great, but difficulties in practice.
  - Must design new representations, operators, tune, ...
- This talk
  - Discuss a promising direction in GEC.
  - Combine machine learning and GEC.
  - Create practical and powerful optimizers.

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## Overview

- Introduction
  - Black-box optimization via probabilistic modeling.
- Probabilistic Model-Building GAs
  - Discrete representation
  - Continuous representation
  - Computer programs (PMBGP)
  - Permutations
- Conclusions

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## Black-box Optimization

- Input
  - How do potential solutions look like?
  - How to evaluate quality of potential solutions?
- Output
  - Best solution (the optimum).
- Important
  - No additional knowledge about the problem.

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## Why View Problem as Black Box?

- Advantages
  - Separate problem definition from optimizer.
  - Easy to solve new problems.
  - Economy argument: BBO saves time & money.
- Difficulties
  - Almost no prior problem knowledge.
  - Problem specifics must be learned automatically.
  - Noise, multiple objectives, interactive evaluation.

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## Representations Considered Here

- Start with
  - Solutions are n-bit binary strings.
- Later
  - Real-valued vectors.
  - Program trees.
  - Permutations

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## Typical Situation in BBO

- Previously visited solutions + their evaluation:

#	Solution	Evaluation
1	00100	1
2	11011	4
3	01101	0
4	10111	3

- Question: What solution to generate next?

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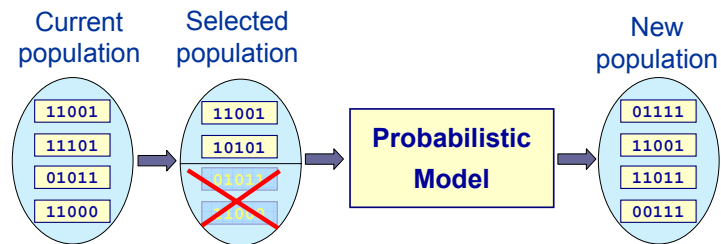
## Many Answers

- Hill climber
  - Start with a random solution.
  - Flip bit that improves the solution most.
  - Finish when no more improvement possible.
- Simulated annealing
  - Introduce Metropolis.
- Probabilistic model-building GAs
  - Inspiration from GAs and machine learning (ML).

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## Probabilistic Model-Building GAs



...replace crossover+mutation with learning and sampling probabilistic model

## Other Names for PMBGAs

- Estimation of distribution algorithms (EDAs) (Mühlenbein & Paass, 1996)
- Iterated density estimation algorithms (IDEA) (Bosman & Thierens, 2000)

## What Models to Use?

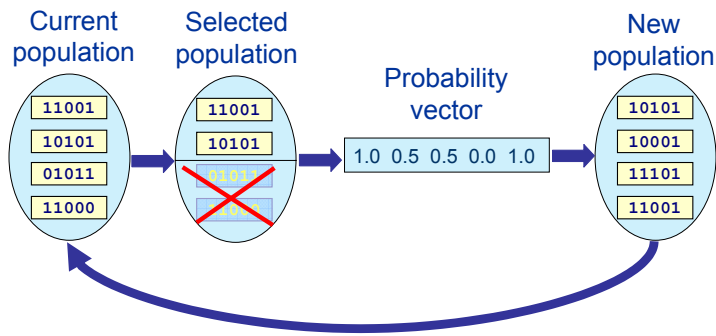
- Start with a simple example
  - Probability vector for binary strings.
- Later
  - Dependency tree models (COMIT).
  - Bayesian networks (BOA).
  - Bayesian networks with local structures (hBOA).

## Probability Vector

- Assume  $n$ -bit binary strings.
- Model: **Probability vector**  $p = (p_1, \dots, p_n)$ 
  - $p_i$  = probability of 1 in position  $i$
  - Learn  $p$ : Compute proportion of 1 in each position.
  - Sample  $p$ : Sample 1 in position  $i$  with prob.  $p_i$

## Example: Probability Vector

(Mühlenbein, Paass, 1996), (Baluja, 1994)



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## Probability Vector PMBGAs

- **PBIL** (Baluja, 1995)
  - Incremental updates to the prob. vector.
- **Compact GA** (Harik, Lobo, Goldberg, 1998)
  - Also incremental updates but better analogy with populations.
- **UMDA** (Mühlenbein, Paass, 1996)
  - What we showed here.
- **DEUM** (Shakya et al., 2004)
- All variants perform similarly.

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## Probability Vector Dynamics

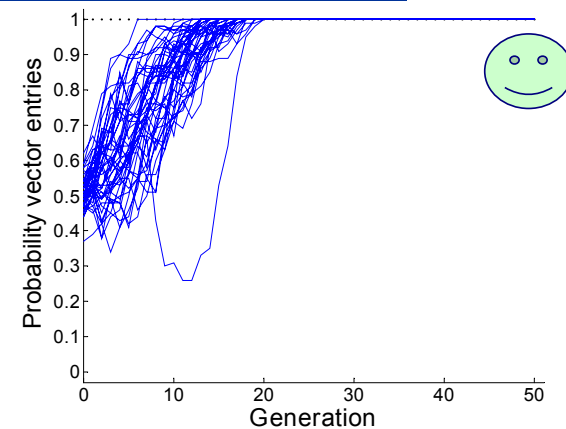
- Bits that perform better get more copies.
- And are combined in new ways.
- But context of each bit is ignored.
- Example problem 1: **Onemax**

$$f(X_1, X_2, \dots, X_n) = \sum_{i=1}^n X_i$$

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## Probability Vector on Onemax



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## Probability Vector: Ideal Scale-up

- $O(n \log n)$  evaluations until convergence
  - (Harik, Cantú-Paz, Goldberg, & Miller, 1997)
  - (Mühlenbein, Schlierkamp-Vosen, 1993)
- Other algorithms
  - Hill climber:  $O(n \log n)$  (Mühlenbein, 1992)
  - GA with uniform: approx.  $O(n \log n)$
  - GA with one-point: slightly slower

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## When Does Prob. Vector Fail?

- Example problem 2: **Concatenated traps**
  - Partition input string into disjoint groups of 5 bits.
  - Groups contribute via trap (ones=number of ones):

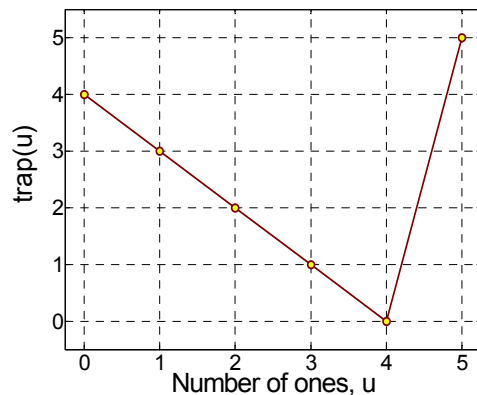
$$\text{trap}(\text{ones}) = \begin{cases} 5 & \text{if } \text{ones} = 5 \\ 4 - \text{ones} & \text{otherwise} \end{cases}$$

- Concatenated trap = sum of single traps
- Optimum: String 111...1

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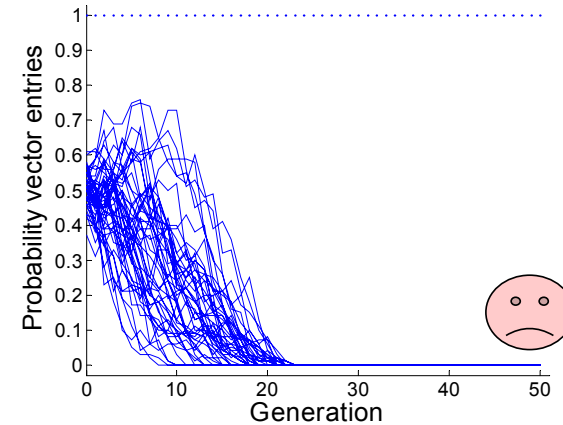
## Trap-5



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## Probability Vector on Traps



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## Why Failure?

- Onemax:
  - Optimum in 111...1
  - 1 outperforms 0 on average.
- Traps: optimum in 11111, but
  - $f(0^{****}) = 2$
  - $f(1^{****}) = 1.375$
- So single bits are misleading.

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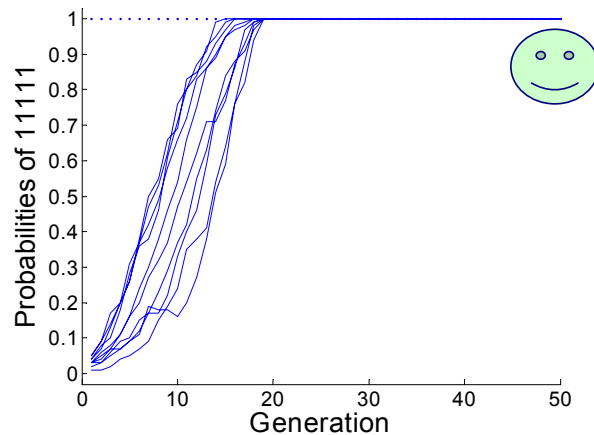
## How to Fix It?

- Consider 5-bit statistics instead 1-bit ones.
- Then, 11111 would outperform 00000.
- Learn model
  - Compute  $p(00000)$ ,  $p(00001)$ , ...,  $p(11111)$
- Sample model
  - Sample 5 bits at a time
  - Generate 00000 with  $p(00000)$ , 00001 with  $p(00001)$ , ...

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## Correct Model on Traps: Dynamics



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## Good News: Good Stats Work Great!

- Optimum in  $O(n \log n)$  evaluations.
- Same performance as on onemax!
- Others
  - Hill climber:  $O(n^5 \log n)$  = much worse.
  - GA with uniform:  $O(2^n)$  = intractable.
  - GA with k-point crossover:  $O(2^n)$  (w/o tight linkage).

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## Challenge

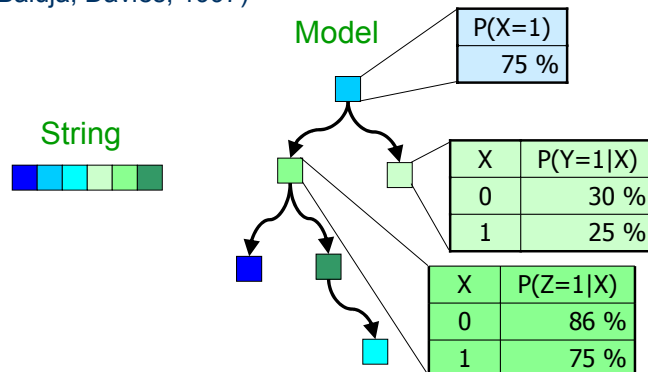
- If we could **learn** and **use** relevant **context** for each position
  - Find nonmisleading statistics.
  - Use those statistics as in probability vector.
- Then we could solve problems decomposable into statistics of order at most  $k$  with at most  $O(n^2)$  evaluations!
  - And there are many such problems (Simon, 1968).

## What's Next?

- COMIT
  - Use tree models
- Extended compact GA
  - Cluster bits into groups.
- Bayesian optimization algorithm (BOA)
  - Use Bayesian networks (more general).

## Beyond single bits: COMIT

(Baluja, Davies, 1997)



## How to Learn a Tree Model?

- Mutual information:

$$I(X_i, X_j) = \sum_{a,b} P(X_i = a, X_j = b) \log \frac{P(X_i = a, X_j = b)}{P(X_i = a)P(X_j = b)}$$

- Goal
  - Find **tree that maximizes mutual information** between connected nodes.
  - Will minimize Kullback-Leibler divergence.
- Algorithm
  - Prim's algorithm for maximum spanning trees.

## Prim's Algorithm

- Start with a graph with no edges.
- Add arbitrary node to the tree.
- Iterate
  - Hang a new node to the current tree.
  - Prefer addition of edges with large mutual information (greedy approach).
- Complexity:  $O(n^2)$

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## Variants of PMBGAs with Tree Models

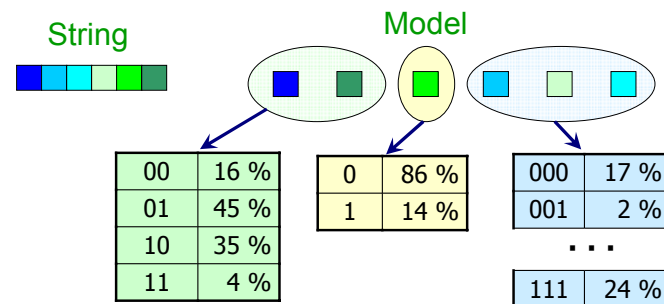
- **COMIT** (Baluja, Davies, 1997)
  - Tree models.
- **MIMIC** (DeBonet, 1996)
  - Chain distributions.
- **BMDA** (Pelikan, Mühlenbein, 1998)
  - Forest distribution (independent trees or tree)

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## Beyond Pairwise Dependencies: ECGA

- Extended Compact GA (ECGA) (Harik, 1999).
- Consider groups of string positions.

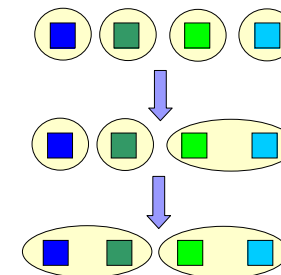


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## Learning the Model in ECGA

- Start with each bit in a separate group.
- Each iteration merges two groups for best improvement.



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## How to Compute Model Quality?

- ECGA uses **minimum description length**.
- Minimize number of bits to store model+data:

$$MDL(M, D) = D_{Model} + D_{Data}$$

- Each frequency needs  $(0.5 \log N)$  bits:

$$D_{Model} = \sum_{g \in G} 2^{|g|-1} \log N$$

- Each solution  $X$  needs  $-\log p(X)$  bits:

$$D_{Data} = -N \sum_X p(X) \log p(X)$$

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## Sampling Model in ECGA

- Sample groups of bits at a time.
- Based on observed probabilities/proportions.
- But can also apply population-based crossover similar to uniform but w.r.t. model.

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## Building-Block-Wise Mutation in ECGA

- Sastry, Goldberg (2004); Lima et al. (2005)
- Basic idea
  - Use ECGA model builder to identify decomposition
  - Use the best solution for BB-wise mutation
  - For each k-bit partition (building block)
    - Evaluate the remaining  $2^{k-1}$  instantiations of this BB
    - Use the best instantiation of this BB
- Result (for order-k separable problems)
  - BB-wise mutation is  $O(\sqrt{k} \log n)$  times faster than ECGA!
  - But only for separable problems (and similar ones).

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## What's Next?

- We saw
  - Probability vector (no edges).
  - Tree models (some edges).
  - Marginal product models (groups of variables).
- Next: Bayesian networks
  - Can represent all above and more.

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## Bayesian Optimization Algorithm (BOA)

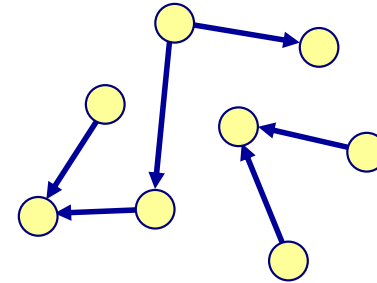
- Pelikan, Goldberg, & Cantú-Paz (1998)
- Use a Bayesian network (BN) as a model.
- Bayesian network
  - Acyclic directed graph.
  - Nodes are variables (string positions).
  - Conditional dependencies (edges).
  - Conditional independencies (implicit).

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## Example: Bayesian Network (BN)

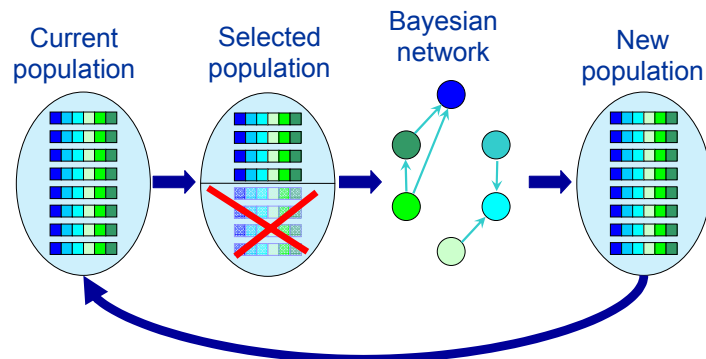
- Conditional dependencies.
- Conditional independencies.



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## BOA



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## Learning BNs

- Two things again:
  - Scoring metric (as MDL in ECGA).
  - Search procedure (in ECGA done by merging).

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## Learning BNs: Scoring Metrics

- Bayesian metrics

- Bayesian-Dirichlet with likelihood equivalence

$$BD(B) = p(B) \prod_{i=1}^n \prod_{\pi_i} \frac{\Gamma(m'(\pi_i))}{\Gamma(m'(\pi_i) + m(\pi_i))} \prod_{x_i} \frac{\Gamma(m'(x_i, \pi_i) + m(x_i, \pi_i))}{\Gamma(m'(x_i, \pi_i))}$$

- Minimum description length metrics

- Bayesian information criterion (BIC)

$$BIC(B) = \sum_{i=1}^n \left( -H(X_i | \Pi_i) N - 2^{|\Pi_i|} \frac{\log_2 N}{2} \right)$$

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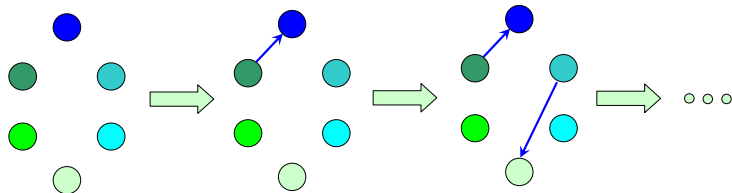
## Learning BNs: Search Procedure

- Start with empty network (like ECGA).
- Execute primitive operator that improves the metric the most (greedy).
- Until no more improvement possible.
- Primitive operators
  - Edge addition (most important).
  - Edge removal.
  - Edge reversal.

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## Learning BNs: Example



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## BOA and Problem Decomposition

- Conditions for factoring problem decomposition into a product of prior and conditional probabilities of small order in Mühlenbein, Mahnig, & Rodriguez (1999).
- In practice, approximate factorization sufficient that can be learned automatically.
- Learning makes complete theory intractable.

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## BOA Theory: Population Sizing

- **Initial supply** (Goldberg et al., 2001)
  - Have enough stuff to combine.  $\Rightarrow O(2^k)$
- **Decision making** (Harik et al, 1997)
  - Decide well between competing partial sols.  $\Rightarrow O(\sqrt{n \log n})$
- **Drift** (Thierens, Goldberg, Pereira, 1998)
  - Don't lose less salient stuff prematurely.  $\Rightarrow O(n)$
- **Model building** (Pelikan et al., 2000, 2002)
  - Find a good model.  $\Rightarrow O(n^{1.05})$

## BOA Theory: Num. of Generations

- Two extreme cases, everything in the middle.
- **Uniform scaling**
  - Onemax model (Muehlenbein & Schlierkamp-Voosen, 1993)

$$O(\sqrt{n})$$

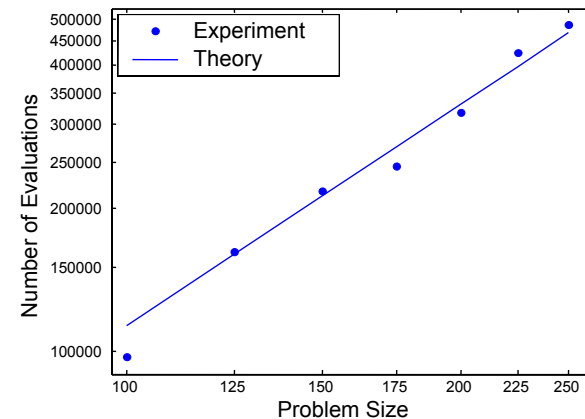
- **Exponential scaling**
  - Domino convergence (Thierens, Goldberg, Pereira, 1998)

$$O(n)$$

## Good News: Challenge Met!

- **Theory**
  - **Population sizing** (Pelikan et al., 2000, 2002)
    - Initial supply.
    - Decision making.  $\Rightarrow O(n) \text{ to } O(n^{1.05})$
    - Drift.
    - Model building.
  - **Number of iterations** (Pelikan et al., 2000, 2002)
    - Uniform scaling.  $\Rightarrow O(n^{0.5}) \text{ to } O(n)$
    - Exponential scaling.
- BOA solves order-k decomposable problems in  $O(n^{1.55})$  to  $O(n^2)$  evaluations!

## Theory vs. Experiment (5-bit Traps)



## BOA Siblings

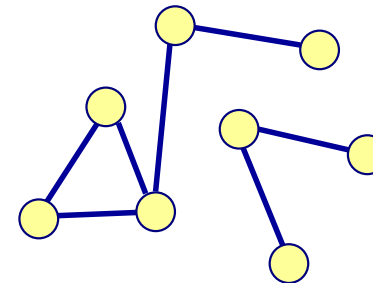
- **Estimation of Bayesian Networks Algorithm (EBNA)** (Etxeberria, Larrañaga, 1999).
- **Learning Factorized Distribution Algorithm (LFDA)** (Mühlenbein, Mahnig, Rodriguez, 1999).

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## Another Option: Markov Networks

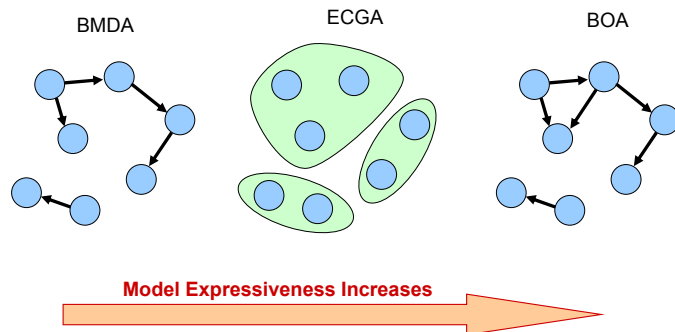
- MN-FDA, MN-EDA (Santana; 2003, 2005)
- Similar to Bayes nets but with undirected edges.



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## Model Comparison



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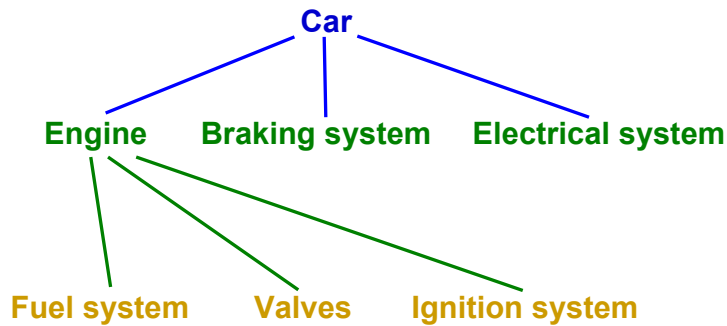
## From single level to hierarchy

- Single-level decomposition powerful.
- But what if single-level decomposition is not enough?
- Learn from humans and nature
  - Decompose problem over multiple levels.
  - Use solutions from lower level as basic building blocks.
  - Solve problem **hierarchically**.

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## Hierarchical Decomposition



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## Three Keys to Hierarchy Success

- **Proper decomposition**
  - Must decompose problem on each level properly.
- **Chunking**
  - Must represent & manipulate large order solutions.
- **Preservation of alternative solutions**
  - Must preserve alternative partial solutions (chunks).

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## Hierarchical BOA (hBOA)

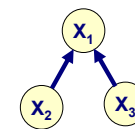
- Pelikan & Goldberg (2000, 2001)
- **Proper decomposition**
  - Use Bayesian networks like BOA.
- **Chunking**
  - Use local structures in Bayesian networks.
- **Preservation of alternative solutions.**
  - Use restricted tournament replacement (RTR).
  - Can use other niching methods.

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## Local Structures in BNs

- Look at one conditional dependency.
  - $2^k$  probabilities for  $k$  parents.
- Why not use more powerful representations for conditional probabilities?



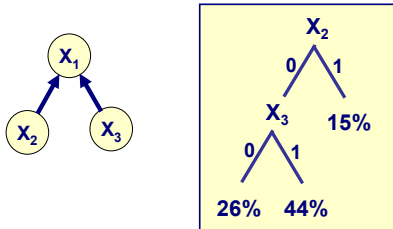
$X_2X_3$	$P(X_1=0 X_2X_3)$
00	26 %
01	44 %
10	15 %
11	15 %

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## Local Structures in BNs

- Look at one conditional dependency.
  - $2^k$  probabilities for  $k$  parents.
- Why not use more powerful representations for conditional probabilities?



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## Restricted Tournament Replacement

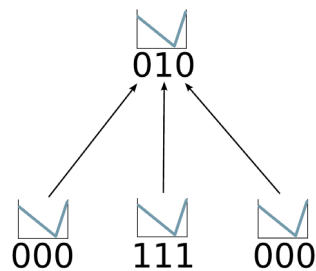
- Used in hBOA for niching.
- Insert each new candidate solution  $x$  like this:
  - Pick random subset of original population.
  - Find solution  $y$  most similar to  $x$  in the subset.
  - Replace  $y$  by  $x$  if  $x$  is better than  $y$ .

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## Hierarchical Traps: The Ultimate Test

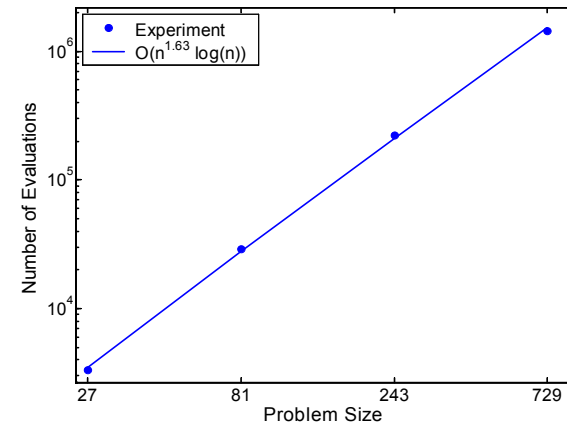
- Combine traps on more levels.
- Each level contributes to fitness.
- Groups of bits map to next level.



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## hBOA on Hierarchical Traps



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## Efficiency Enhancement for PMBGAs

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- Sometimes  $O(n^2)$  is not enough
  - High-dimensional problems (1000s of variables)
  - Expensive evaluation (fitness) function
- Solution
  - Efficiency enhancement techniques

## Efficiency Enhancement Types

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- **7 efficiency enhancement types** for PMBGAs
  - Parallelization
  - Hybridization
  - Time continuation
  - Fitness evaluation relaxation
  - Prior knowledge utilization
  - Incremental and sporadic model building
  - Learning from experience

## Multi-objective PMBGAs

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- Methods for multi-objective GAs adopted
  - Multi-objective hBOA (from NSGA-II and hBOA) (Khan, Goldberg, & Pelikan, 2002) (Pelikan, Sastry, & Goldberg, 2005)
  - Another multi-objective BOA (from SPEA2) (Laumanns, & Ocenasek, 2002)
  - Multi-objective mixture-based IDEAs (Thierens, & Bosman, 2001)

## Promising Results with Discrete PMBGAs

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- Artificial classes of problems
- Physics
- Computational complexity and AI
- Others



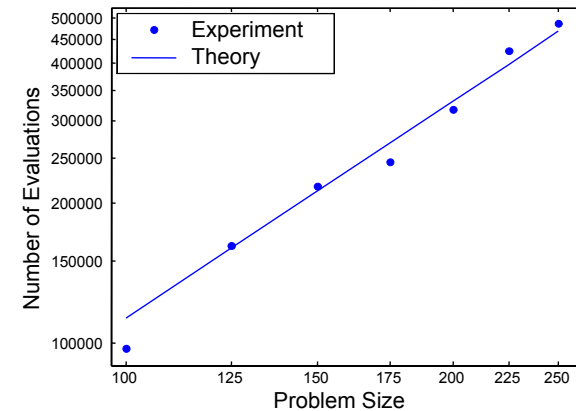
## Results: Artificial Problems

- Decomposition
  - Concatenated traps (Pelikan et al., 1998).
- Hierarchical decomposition
  - Hierarchical traps (Pelikan, Goldberg, 2001).
- Other sources of difficulty
  - Exponential scaling, noise (Pelikan, 2002).

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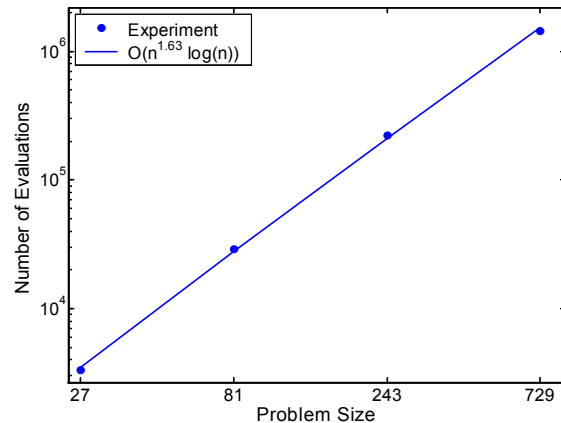
## BOA on Concatenated 5-bit Traps



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## hBOA on Hierarchical Traps



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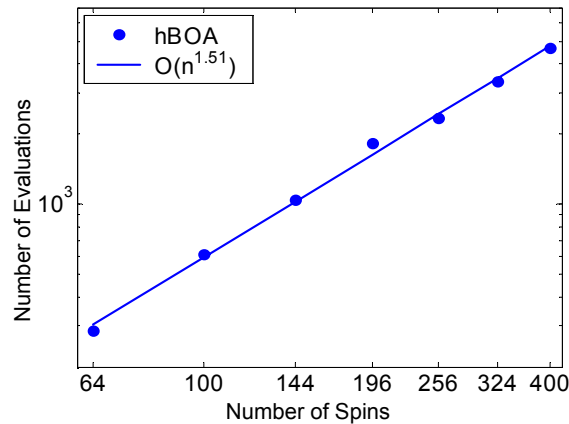
## Results: Physics

- Spin glasses (Pelikan, 2002)
  - $\pm J$  and Gaussian couplings
  - 2D and 3D
- Silicon clusters (Sastry, 2001)
  - Gong potential (3-body)

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## hBOA on Ising Spin Glasses (2D)



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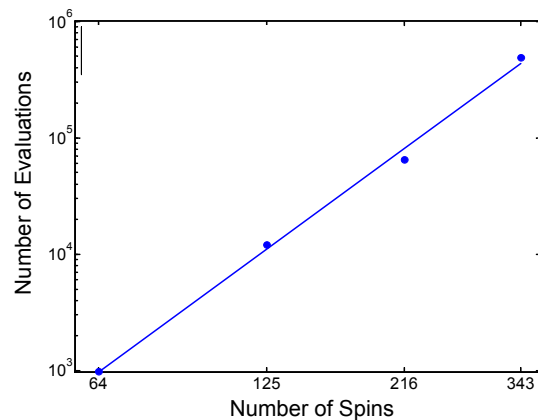
## Results on 2D Spin Glasses

- Number of evaluations is  $O(n^{1.51})$ .
- Overall time is  $O(n^{3.51})$ .
- Compare  $O(n^{3.51})$  to  $O(n^{3.5})$  for best method (Galluccio & Loeb, 1999)
- Great also on Gaussians.

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## hBOA on Ising Spin Glasses (3D)



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## Results: Computational Complexity, AI

- MAXSAT, SAT (Pelikan, 2002)
  - Random 3CNF from phase transition.
  - Morphed graph coloring.
  - Conversion from spin glass.
- Feature subset selection (Inza et al., 2001) (Cantu-Paz, 2004)

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## Results: Some Others

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- Military antenna design (Santarelli et al., 2004)
- Groundwater remediation design (Arst et al., 2004)
- Forest management (Ducheyne et al., 2003)
- Nurse scheduling (Li, Aickelin, 2004)
- Telecommunication network design (Rothlauf, 2002)
- Graph partitioning (Ocenasek, Schwarz, 1999; Muehlenbein, Mahnig, 2002; Baluja, 2004)
- Portfolio management (Lipinski, 2005, 2007)
- Quantum excitation chemistry (Sastry et al., 2005)
- Minimum vertex cover (Pelikan et al., 2007)

## Discrete PMBGAs: Summary

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- No interactions
  - Univariate models; PBIL, UMDA, cGA.
- Some pairwise interactions
  - Tree models; COMIT, MIMIC, BMDA.
- Multivariate interactions
  - Multivariate models: BOA, EBNA, LFDA.
- Hierarchical decomposition
  - hBOA

## Discrete PMBGAs: Recommendations

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- Easy problems
  - Use univariate models; PBIL, UMDA, cGA.
- Somewhat difficult problems
  - Use bivariate models; MIMIC, COMIT, BMDA.
- Difficult problems
  - Use multivariate models; BOA, EBNA, LFDA.
- Most difficult problems
  - Use hierarchical decomposition; hBOA.

## Continuous PMBGAs

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- New challenge
  - Infinite domain for each variable.
  - How to model?
- 2 approaches
  - Discretize and apply discrete model/PMBGA
  - Create continuous model
    - Estimate pdf.

## PBIL Extensions: First Step

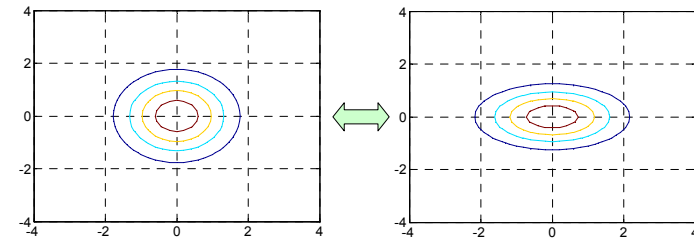
- SHCwL: Stochastic hill climbing with learning (Rudlof, Köppen, 1996).
- Model
  - Single-peak Gaussian for each variable.
  - Means evolve based on parents (promising solutions).
  - Deviations equal, decreasing over time.
- Problems
  - No interactions.
  - Single Gaussians=can model only one attractor.
  - Same deviations for each variable.

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## Use Different Deviations

- Sebag, Ducoulombier (1998)
- Some variables have higher variance.
- Use special standard deviation for each variable.

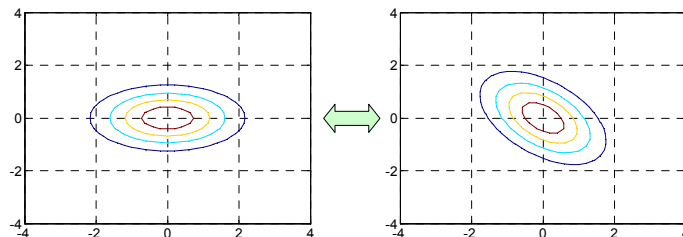


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## Use Covariance

- Covariance allows rotation of 1-peak Gaussians.
- EGNA (Larrañaga et al., 2000)
- IDEA (Bosman, Thierens, 2000)

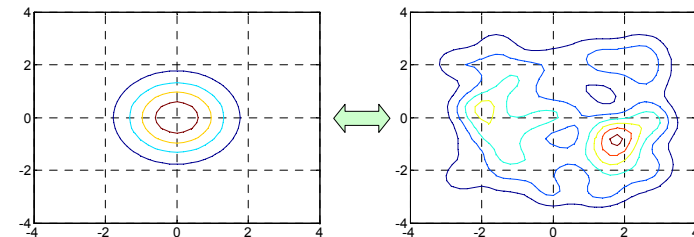


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## How Many Peaks?

- One Gaussian vs. kernel around each point.
- Kernel distribution similar to ES.
- IDEA (Bosman, Thierens, 2000)

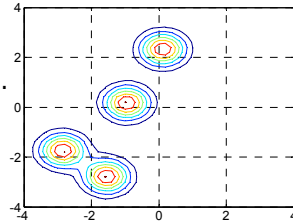


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## Mixtures: Between One and Many

- Mixture distributions provide transition between one Gaussian and Gaussian kernels.
- Mixture types
  - Over one variable.
    - Gallagher, Frenn, & Downs (1999).
  - Over all variables.
    - Pelikan & Goldberg (2000).
    - Bosman & Thierens (2000).
  - Over partitions of variables.
    - Bosman & Thierens (2000).
    - Ahn, Ramakrishna, and Goldberg (2004).



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## Mixed BOA (mBOA)

- Mixed BOA (Ocenasek, Schwarz, 2002)
- Local distributions
  - A decision tree (DT) for every variable.
  - Internal DT nodes encode tests on other variables
    - Discrete: Equal to a constant
    - Continuous: Less than a constant
  - Discrete variables: DT leaves represent probabilities.
  - Continuous variables: DT leaves contain a normal kernel distribution.

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## Real-Coded BOA (rBOA)

- Ahn, Ramakrishna, Goldberg (2003)
- Probabilistic Model
  - Underlying structure: Bayesian network
  - Local distributions: Mixtures of Gaussians
- Also extended to multiobjective problems (Ahn, 2005)

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## Aggregation Pheromone System (APS)

- Tsutsui (2004)
- Inspired by aggregation pheromones
- Basic idea
  - Good solutions emit aggregation pheromones
  - New candidate solutions based on the density of aggregation pheromones
  - Aggregation pheromone density encodes a mixture distribution

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## Continuous PMBGAs: Discretization

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- Idea: Transform into discrete domain.
- Fixed models
  - $2^k$  equal-width bins with k-bit binary string.
  - Goldberg (1989).
  - Bosman & Thierens (2000); Pelikan et al. (2003).
- Adaptive models
  - Equal-height histograms of  $2k$  bins.
  - k-means clustering on each variable.
  - Pelikan, Goldberg, & Tsutsui (2003); Cantu-Paz (2001).

## Continuous PMBGAs: Summary

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- Discretization
  - Fixed
  - Adaptive
- Continuous models
  - Single or multiple peaks?
  - Same variance or different variance?
  - Covariance or no covariance?
  - Mixtures?
  - Treat entire vectors, subsets of variables, or single variables?

## Continuous PMBGAs: Recommendations

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- Multimodality?
  - Use multiple peaks.
- Decomposability?
  - All variables, subsets, or single variables.
- Strong linear dependencies?
  - Covariance.
- Partial differentiability?
  - Combine with gradient search.

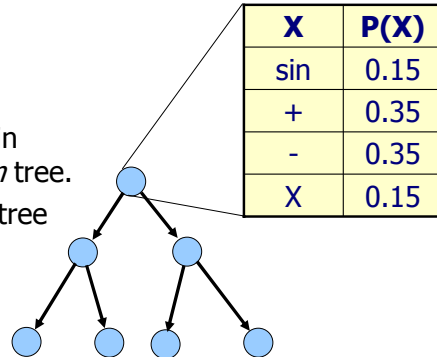
## PMBGP (Genetic Programming)

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- New challenge
  - Structured, variable length representation.
  - Possibly infinitely many values.
  - Position independence (or not).
  - Low correlation between solution quality and solution structure (Looks, 2006).
- Approaches
  - Use explicit probabilistic models for trees.
  - Use models based on grammars.

## PIPE

- Probabilistic incremental program evolution (Salustowicz & Schmidhuber, 1997)
- Store frequencies of operators/terminals in nodes of a *maximum* tree.
- Sampling generates tree from top to bottom

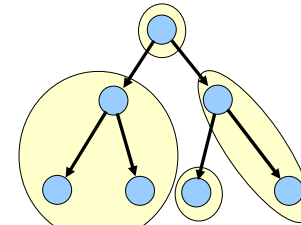


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## eCGP

- Sastry & Goldberg (2003)
- ECGA adapted to program trees.
- Maximum tree as in PIPE.
- But nodes partitioned into groups.



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## BOA for GP

- Looks, Goertzel, & Pennachin (2004)
- Combinatory logic + BOA
  - Trees translated into uniform structures.
  - Labels only in leaves.
  - BOA builds model over symbols in different nodes.
- Complexity build-up
  - Modeling limited to max. sized structure seen.
  - Complexity builds up by special operator.

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## MOSES

- Looks (2006).
- Evolve demes of programs.
- Each deme represents similar structures.
- Apply PMBGA to each deme (e.g. hBOA).
- Introduce new demes/delete old ones.
- Use normal forms to reduce complexity.

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## PMBGP with Grammars

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- Use grammars/stochastic grammars as models.
- Grammars restrict the class of programs.
  
- Some representatives
  - Program evolution with explicit learning (Shan et al., 2003)
  - Grammar-based EDA for GP (Bosman, de Jong, 2004)
  - Stochastic grammar GP (Tanev, 2004)
  - Adaptive constrained GP (Janikow, 2004)

## PMBGP: Summary

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- Interesting starting points available.
- But still lot of work to be done.
- Much to learn from discrete domain, but some completely new challenges.
- Research in progress

## PMBGAs for Permutations

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- New challenges
  - Relative order
  - Absolute order
  - Permutation constraints
- Two basic approaches
  - Random-key and real-valued PMBGAs
  - Explicit probabilistic models for permutations

## Random Keys and PMBGAs

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- Bengoetxea et al. (2000); Bosman et al. (2001)
- Random keys (Bean, 1997)
  - Candidate solution = vector of real values
  - Ascending ordering gives a permutation
- Can use any real-valued PMBGA (or GEA)
  - IDEAs (Bosman, Thierens, 2002)
  - EGNA (Larranaga et al., 2001)
- Strengths and weaknesses
  - Good: Can use any real-valued PMBGA.
  - Bad: Redundancy of the encoding.



## Direct Modeling of Permutations

- Edge-histogram based sampling algorithm (EHBSA) (Tsutsui, Pelikan, Goldberg, 2003)
  - Permutations of  $n$  elements
  - Model is a matrix  $A=(a_{i,j})_{i,j=1, 2, \dots, n}$
  - $a_{i,j}$  represents the probability of edge  $(i, j)$
  - Uses template to reduce exploration
  - Applicable also to scheduling

## Multivariate Permutation Models

- Basic approach
  - Use any standard multivariate discrete model.
  - Restrict sampling to permutations in some way.
  - Bengoetxea et al. (2000), Pelikan et al. (2007).
- Strengths and weaknesses
  - Use explicit multivariate models to find regularities.
  - High-order alphabet requires big samples for good models.
  - Sampling can introduce unwanted bias.
  - Inefficient encoding for only relative ordering constraints, which can be encoded simpler.

## Conclusions

- Competent PMBGAs exist
  - Scalable solution to broad classes of problems.
  - Solution to previously intractable problems.
  - Algorithms ready for new applications.
- Consequences for practitioners
  - Robust methods with few or no parameters.
  - Capable of learning how to solve problem.
  - But can incorporate prior knowledge as well.
  - Can solve previously intractable problems.

## Starting Points

- World wide web
- Books and surveys
  - Larrañaga & Lozano (eds.) (2001). *Estimation of distribution algorithms: A new tool for evolutionary computation*. Kluwer.
  - Pelikan et al. (2002). *A survey to optimization by building and using probabilistic models*. Computational optimization and applications, 21(1), pp. 5-20.
  - Pelikan (2005). *Hierarchical BOA: Towards a New Generation of Evolutionary Algorithms*. Springer.
  - Lozano, Larrañaga, Inza, Bengoetxea (2007). *Towards a New Evolutionary Computation: Advances on Estimation of Distribution Algorithms*, Springer.
  - Pelikan, Sastry, Cantu-Paz (eds.) (2007). *Scalable Optimization via Probabilistic Modeling: From Algorithms to Applications*, Springer.

### Code

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- BOA, BOA with decision graphs, dependency-tree EDA  
<http://medal.cs.umsl.edu/>
- ECGA, BOA, and BOA with decision trees/graphs  
<http://www-illigal.ge.uiuc.edu/>
- mBOA  
<http://jiri.ocenasek.com/>
- PIPE  
<http://www.idsia.ch/~rafal/>
- Real-coded BOA  
<http://www.evolution.re.kr/>
- Demos of APS and EHBSA  
<http://www.hannan-u.ac.jp/~tsutsui/research-e.html>