

Probabilistic Model-Building Genetic Algorithms

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

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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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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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Problem Formulation

- 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.
- Difficulties
 - Almost no prior problem knowledge.
 - Problem specifics must be learned automatically.
 - Noise, multiple objectives, interactive evaluation.

Typical Situation

- 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?

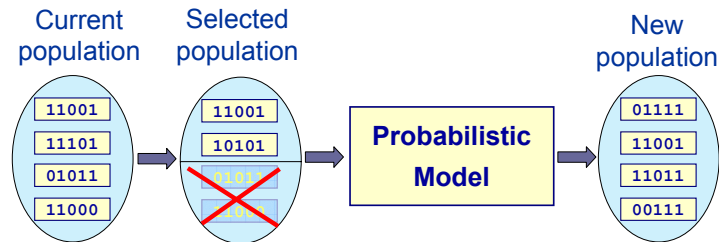
Representations Considered Here

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

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

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).

Other Names for PMBGAs

- Estimation of distribution algorithms (EDAs)
(Mühlenbein & Paass, 1996)

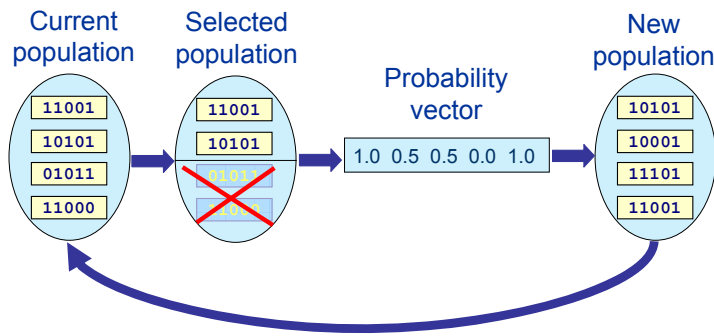
- Iterated density estimation algorithms (IDEA)
(Bosman & Thierens, 2000)

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 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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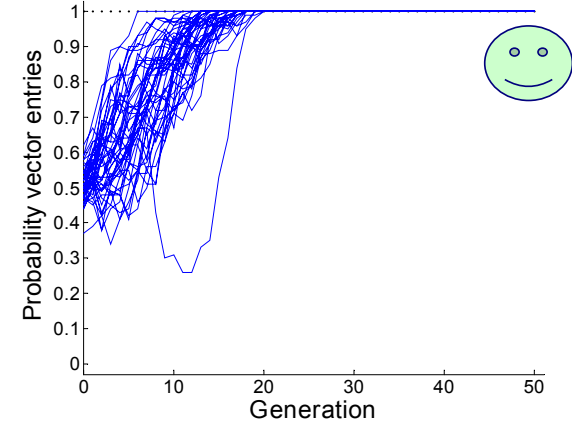
Probability Vector PMBGAs

- **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 on Onemax



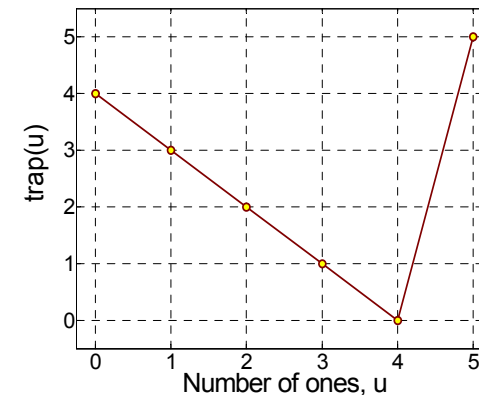
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Probability Vector: Ideal Scale-up

- $O(n \log n)$ 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

Trap-5



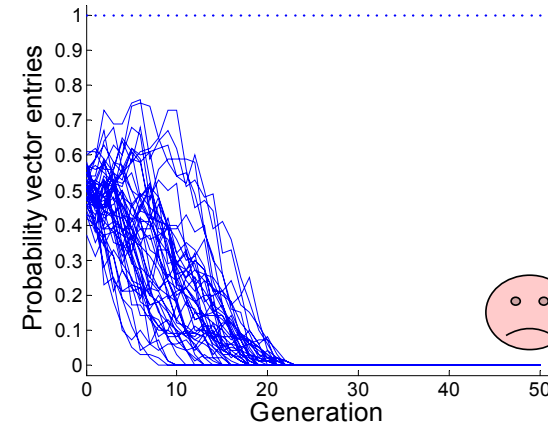
When Does Prob. Vector Fail?

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

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

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

Probability Vector on Traps



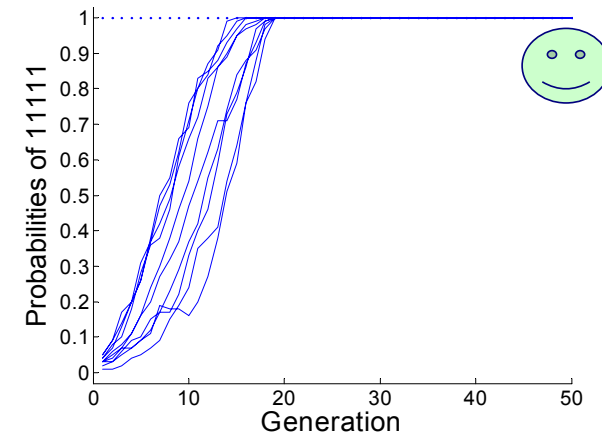
Why Failure?

- 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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Correct Model on Traps: Dynamics



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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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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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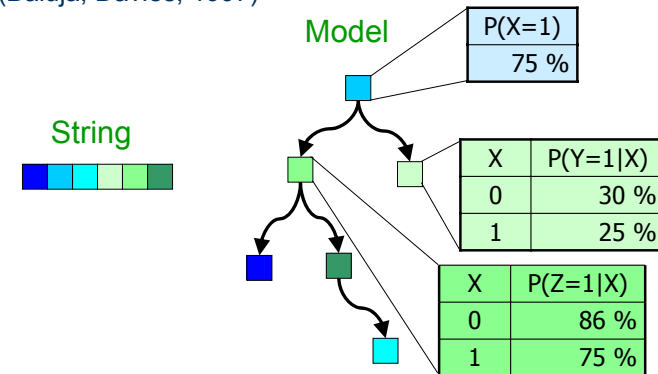
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Challenge

- If we could **learn and use relevant context** for each position
 - Find non-misleading 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).

Beyond single bits: COMIT

(Baluja, Davies, 1997)



What's Next?

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

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

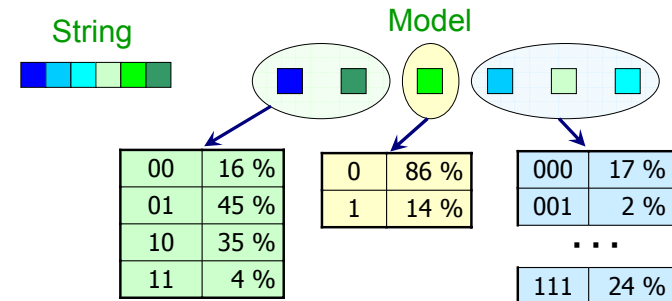
- Start with a graph with no edges.
- Add arbitrary node to the tree.
- Iterate
 - Hang a new node to the current tree.
 - Prefer addition of edges with large mutual information (greedy approach).
- Complexity: $O(n^2)$

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Beyond Pairwise Dependencies: ECGA

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



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Variants of PMBGAs with Tree Models

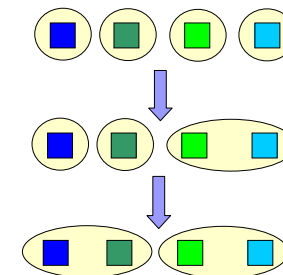
- **COMIT** (Baluja, Davies, 1997)
 - Tree models.
- **MIMIC** (DeBonet, 1996)
 - Chain distributions.
- **BMDA** (Pelikan, Mühlenbein, 1998)
 - Forest distribution (independent trees or tree)

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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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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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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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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.

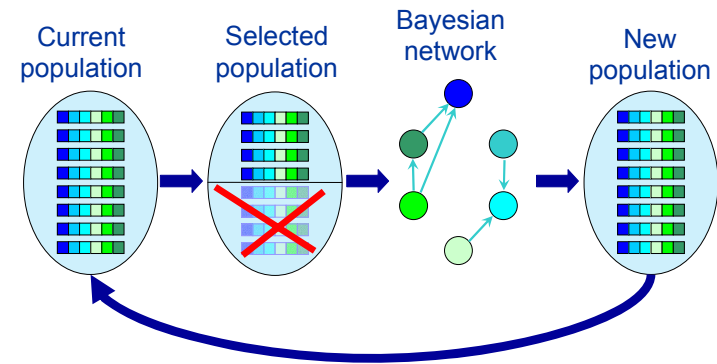
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Bayesian Optimization Algorithm (BOA)

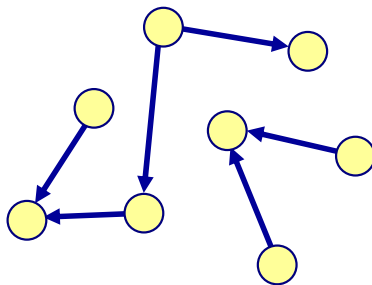
- Pelikan, Goldberg, & Cantú-Paz (1998)
- Use a Bayesian network (BN) as a model.
- Bayesian network
 - Acyclic directed graph.
 - Nodes are variables (string positions).
 - Conditional dependencies (edges).
 - Conditional independencies (implicit).

BOA



Example: Bayesian Network (BN)

- Conditional dependencies.
- Conditional independencies.



Learning BNs

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

Learning BNs: Scoring Metrics

- Bayesian metrics

- Bayesian-Dirichlet with likelihood equivalence

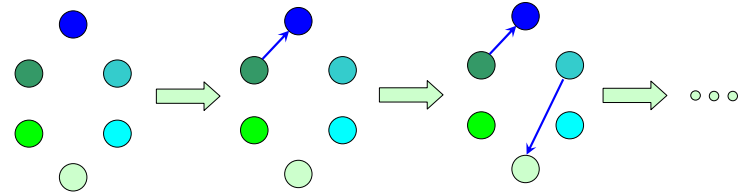
$$BD(B) = p(B) \prod_{i=1}^n \prod_{\pi_i} \frac{\Gamma(m'(\pi_i))}{\Gamma(m'(\pi_i) + m(\pi_i))} \prod_{x_i} \frac{\Gamma(m'(x_i, \pi_i) + m(x_i, \pi_i))}{\Gamma(m'(x_i, \pi_i))}$$

- Minimum description length metrics

- Bayesian information criterion (BIC)

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

Learning BNs: Example



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.

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.

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. $\Rightarrow O(n^{1.05})$

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!**

BOA Theory: Num. of Generations

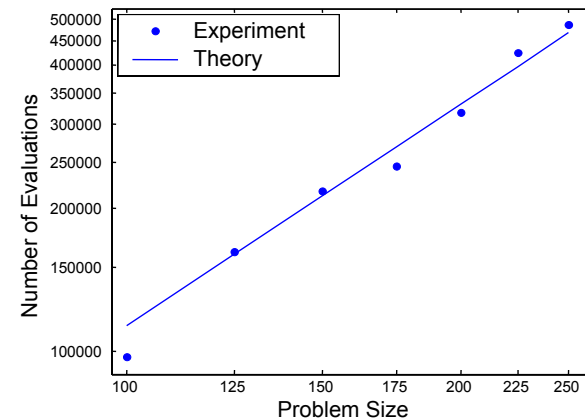
- Two extreme cases, everything in the middle.
- **Uniform scaling**
 - Onemax model (Muehlenbein & Schlierkamp-Voosen, 1993)

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

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

$$O(n)$$

Theory vs. Experiment (5-bit Traps)



BOA Siblings

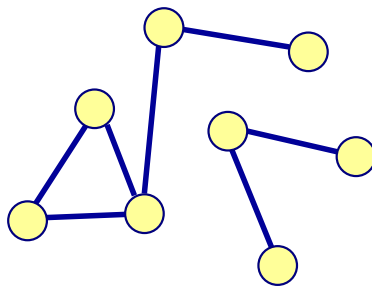
- Estimation of Bayesian Networks Algorithm (EBNA) (Etxeberria, Larrañaga, 1999).
- Learning Factorized Distribution Algorithm (LFDA) (Mühlenbein, Mahnig, Rodriguez, 1999).

Yet Another Option: Dependency Networks

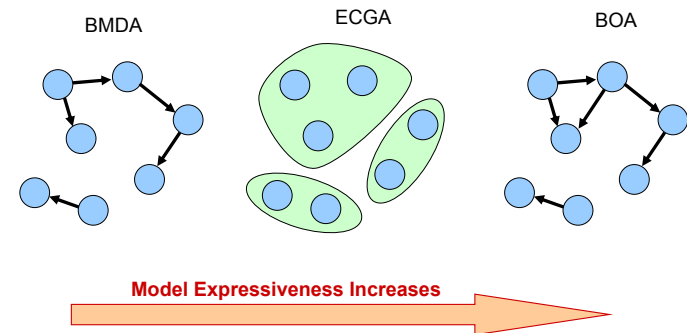
- Estimation of dependency networks algorithm (EDNA)
 - Gamez, Mateo, Puerta (2007).
 - Use dependency network as a model.
 - Dependency network learned from pairwise interactions.
 - Use Gibbs sampling to generate new solutions.
- Dependency network
 - Parents of a variable= all variables influencing this variable.
 - Dependency network can contain cycles.

Another Option: Markov Networks

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



Model Comparison



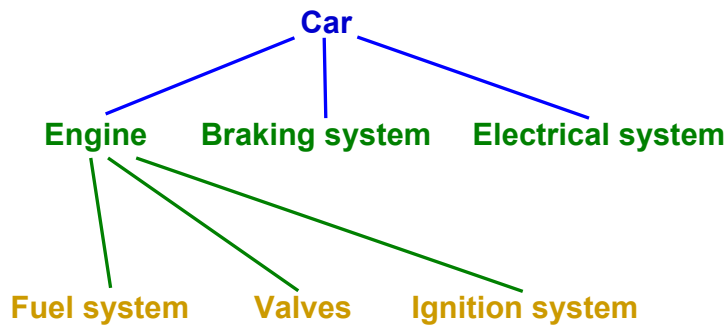
From single level to hierarchy

- 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**.

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).

Hierarchical Decomposition

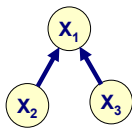


Hierarchical BOA (hBOA)

- 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.

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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Restricted Tournament Replacement

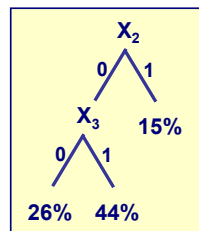
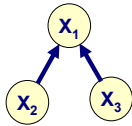
- Used in hBOA for niching.
- Insert each new candidate solution x like this:
 - Pick random subset of original population.
 - Find solution y most similar to x in the subset.
 - Replace y by x if x is better than y .

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Local Structures in BNs

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

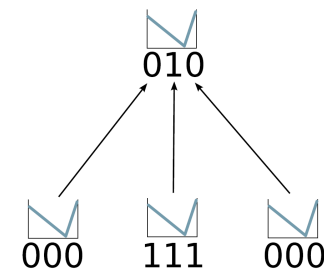


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Hierarchical Traps: The Ultimate Test

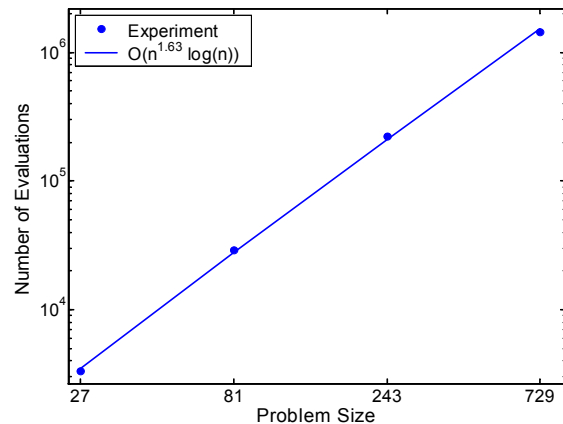
- Combine traps on more levels.
- Each level contributes to fitness.
- Groups of bits map to next level.



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hBOA on Hierarchical Traps



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Efficiency Enhancement for PMBGAs

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

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PMBGAs Are **Not** Just Optimizers

- PMBGAs provide us with two things
 - Optimum or its approximation.
 - Sequence of probabilistic models.
- Probabilistic models
 - Encode populations of increasing quality.
 - Tell us a lot about the problem at hand.
 - Can we use this information?

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Efficiency Enhancement Types

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

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Multi-objective PMBGAs

- 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)
 - Regularity Model Based Multiobjective EDA (RM-MEDA) (Zhang, Zhou, Jin, 2008)

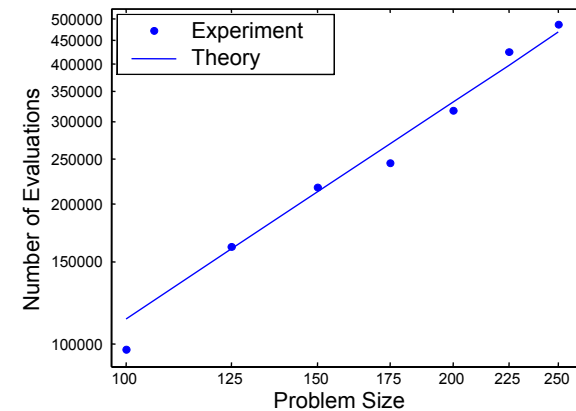
Results: Artificial Problems

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

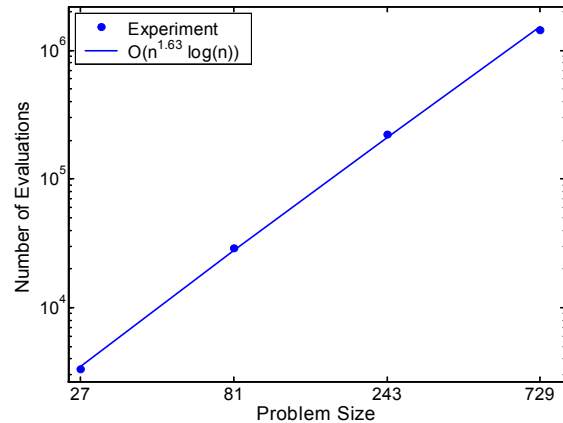
Promising Results with Discrete PMBGAs

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

BOA on Concatenated 5-bit Traps



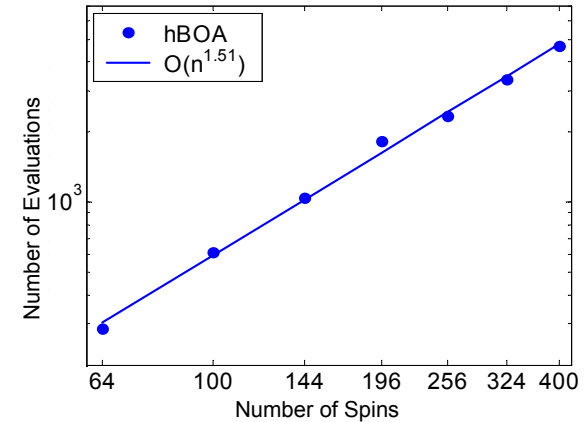
hBOA on Hierarchical Traps



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hBOA on Ising Spin Glasses (2D)



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Results: Physics

- Spin glasses (Pelikan et al., 2002, 2006, 2008) (Hoens, 2005) (Santana, 2005) (Shakya et al., 2006)
 - ±J and Gaussian couplings
 - 2D and 3D spin glass
 - Sherrington-Kirkpatrick (SK) spin glass
- Silicon clusters (Sastry, 2001)
 - Gong potential (3-body)

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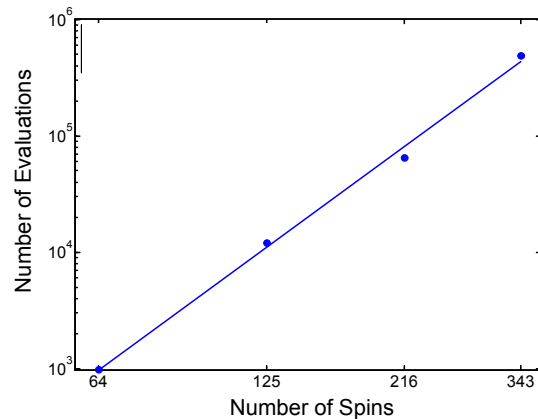
Results on 2D Spin Glasses

- 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 & Loebli, 1999)
- Great also on Gaussians.

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hBOA on Ising Spin Glasses (3D)



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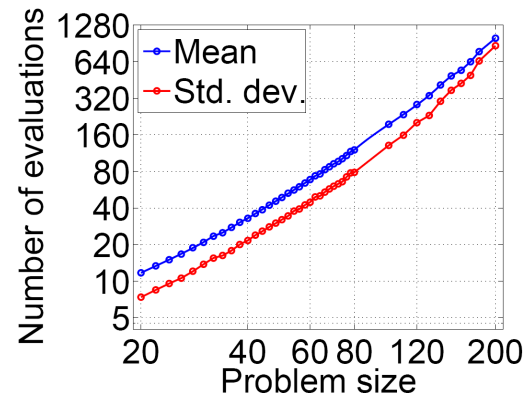
Results: Computational Complexity, AI

- 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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hBOA on SK Spin Glass



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Results: Some Others

- 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)
- Maximum clique (Zhang et al., 2005)
- Cancer chemotherapy optimization (Petrovski et al., 2006)
- Minimum vertex cover (Pelikan et al., 2007)
- Protein folding (Santana et al., 2007)
- Side chain placement (Santana et al., 2007)

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Discrete PMBGAs: Summary

- 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

Real-Valued PMBGAs

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

Discrete PMBGAs: Recommendations

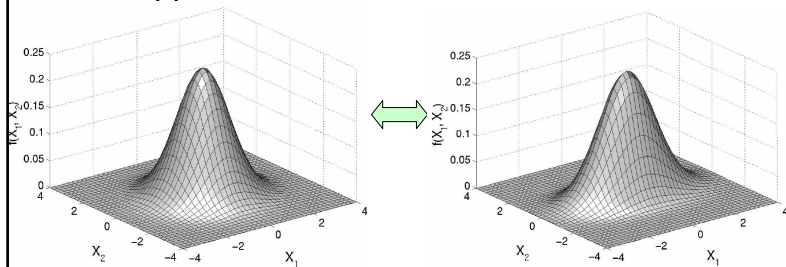
- Easy problems
 - Use univariate models; PBIL, UMDA, cGA.
- Somewhat difficult problems
 - Use bivariate models; MIMIC, COMIT, BMDA.
- Difficult problems
 - Use multivariate models; BOA, EBNA, LFDA.
- Most difficult problems
 - Use hierarchical decomposition; hBOA.

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.

Use Different Deviations

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

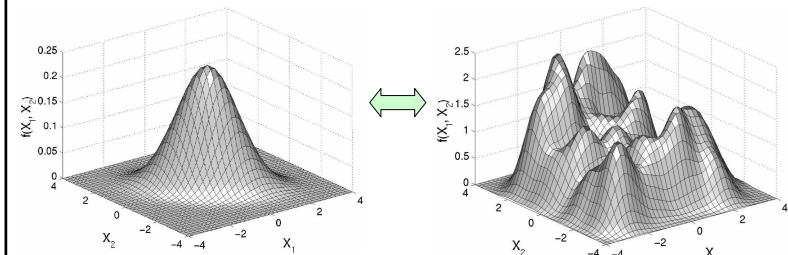


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How Many Peaks?

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

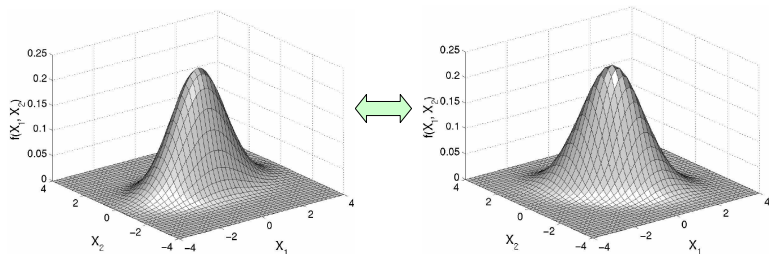


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Use Covariance

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

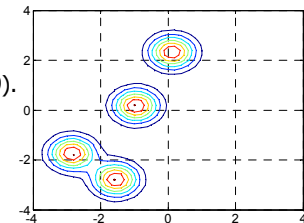


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Mixtures: Between One and Many

- Mixture distributions provide transition between one Gaussian and Gaussian kernels.
- Mixture types
 - Over one variable.
 - Gallagher, Fren, & 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.

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

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)

Adaptive Variance Scaling

- Adaptive variance in mBOA
 - Ocenasek et al. (2004)
- Normal IDEAs
 - Bosman et al. (2006, 2007)
 - Correlation-triggered adaptive variance scaling
 - Standard-deviation ratio (SDR) triggered variance scaling

Real-Valued PMBGAs: Discretization

- 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).

Real-Valued PMBGAs: Recommendations

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

Real-Valued PMBGAs: Summary

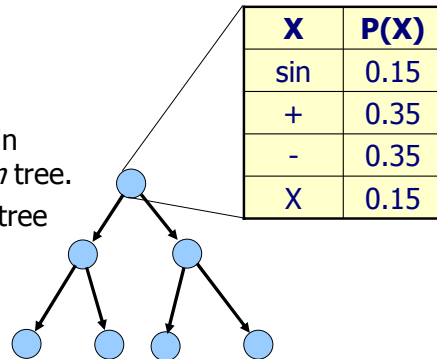
- Discretization
 - Fixed
 - Adaptive
- Real-valued models
 - Single or multiple peaks?
 - Same variance or different variance?
 - Covariance or no covariance?
 - Mixtures?
 - Treat entire vectors, subsets of variables, or single variables?

PMBGP (Genetic Programming)

- 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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BOA for GP

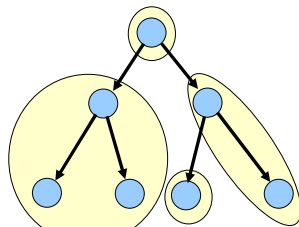
- Looks, Goertzel, & Pennachin (2004)
- Combinatory logic + BOA
 - Trees translated into uniform structures.
 - Labels only in leaves.
 - BOA builds model over symbols in different nodes.
- Complexity build-up
 - Modeling limited to max. sized structure seen.
 - Complexity builds up by special operator.

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eCGP

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



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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

- 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)

PMBGAs for Permutations

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

PMBGP: Summary

- 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

Random Keys and PMBGAs

- 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

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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.

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ICE: Modify Crossover from Model

- ICE
 - Bosman, Thierens (2001).
 - Represent permutations with random keys.
 - Learn multivariate model to factorize the problem.
 - Use the learned model to modify crossover.
- Performance
 - Typically outperforms IDEAs and other PMBGAs that learn and sample random keys.

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Conclusions

- Competent PMBGAs exist
 - Scalable solution to broad classes of problems.
 - Solution to previously intractable problems.
 - Algorithms ready for new applications.
- PMBGAs do more than just solve the problem
 - They provide us with sequences of probabilistic models.
 - The probabilistic models tell us a lot about the problem.
- 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.

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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.

Online Code (2/2)

- Demos of APS and EHBSA
<http://www.hannan-u.ac.jp/~tsutsui/research-e.html>
- RM-MEDA: A Regularity Model Based Multiobjective EDA
Differential Evolution + EDA hybrid
<http://cswwww.essex.ac.uk/staff/qzhang/mypublication.htm>
- Naive Multi-objective Mixture-based IDEA (MIDEA)
Normal IDEA-Induced Chromosome Elements Exchanger (ICE)
Normal Iterated Density-Estimation Evolutionary Algorithm (IDEA)
<http://homepages.cwi.nl/~bosman/code.html>

Online Code (1/2)

- BOA, BOA with decision graphs, dependency-tree EDA
<http://medal.cs.umsl.edu/>
- ECGA, xi-ary 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/>