Probabilistic Model-Building Genetic Algorithms

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Foreword

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

Overview

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

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.

Why View Problem as Black Box?

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

Representations Considered Here

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

Typical Situation in BBO

- Previously visited solutions and their evaluation:

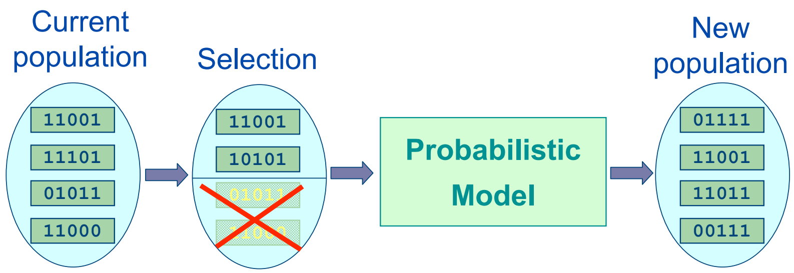
#	Solution	Evaluation
1	00100	1
2	11011	4
3	01101	0
4	10111	3

- Question: What solution to generate next?

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).

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?

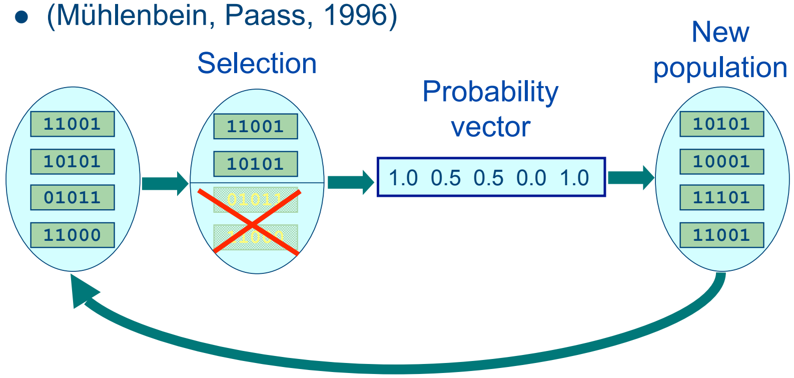
- Start with a simple example
  - Probability vector for binary strings.
- Later
  - Dependency tree models (COMIT).
  - Bayesian networks (BOA).
  - Bayesian networks with local structures (hBOA).

Probability Vector

- Assume n-bit binary strings.
- Model: Probability vector $p=(p_1, \ldots, p_n)$
  - 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)



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.
- All variants perform similarly.

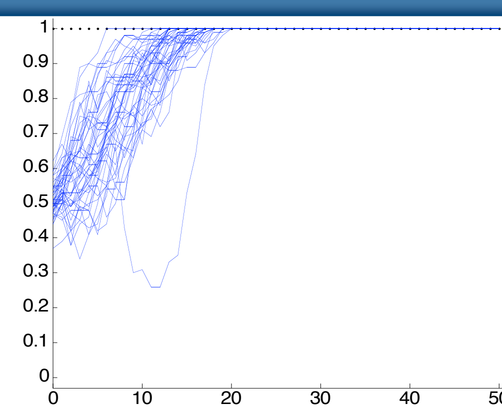
Probability Vector Dynamics

- Bits that perform better get more copies.
- And are combined in new ways.
- But context of each bit is ignored.

- Example problem 1: ONEMAX

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

Probability Vector on ONEMAX



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

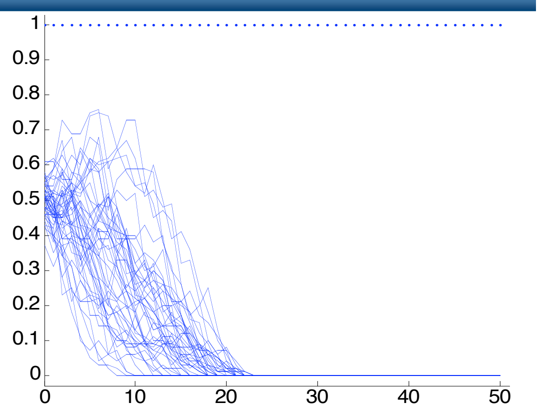
When Does Prob. Vector Fail?

- Example problem 2: Concatenated traps
  - Partition input string into disjoint groups of 5 bits.
  - Each group contributes 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



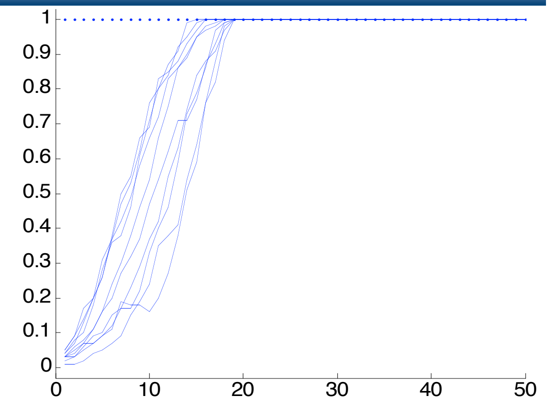
Why Failure?

- 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.

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), …

Correct Model on Traps: Dynamics



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 one point: $O(2^n)$ (without tight linkage).

Challenge

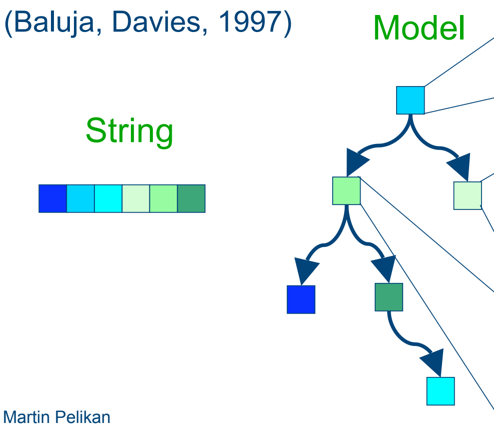
- If we could *learn* and *use* context for each position
  - Find nonmisleading statistics.
  - Use those statistics as in probability vector.
- Then we could solve problems decomposable into statistics of order at most *k* with at most $O(n^2)$ evaluations!
  - And there are many of those problems.

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)



P(X=1)
75 %

X	P(Y=1|X)
0	30 %
1	25 %

X	P(Z=1|X)
0	86 %
1	75 %

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.
- Algorithm
  - Prim’s algorithm for maximum spanning trees.

Prim’s Algorithm

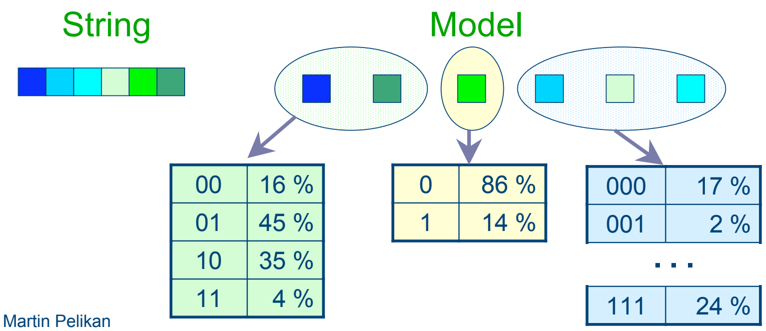
- Start with a graph with no edges.
- Add arbitrary node to the tree.
- Iterate
  - Hang a new node to the tree to any node that maximizes mutual information.
- Complexity: $O(n^2)$

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)

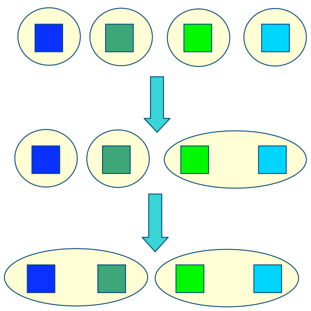
Beyond Pairwise Dependencies: ECGA

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



Learning the Model in ECGA

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



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:

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

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.

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 $O\left(\sqrt{k}\log n\right)$ faster than ECGA.

Next

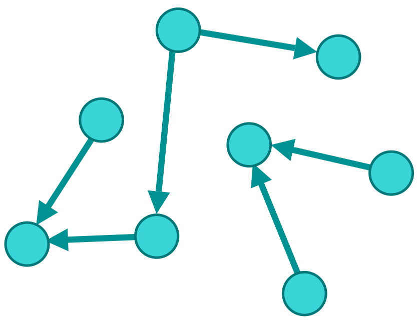
- We saw
  - Probability vector (no edges).
  - Tree models (some edges).
  - Marginal product models (groups of variables).
- Next: Bayesian networks
  - Can represent all above and more.

Bayesian Optimization Algorithm (BOA)

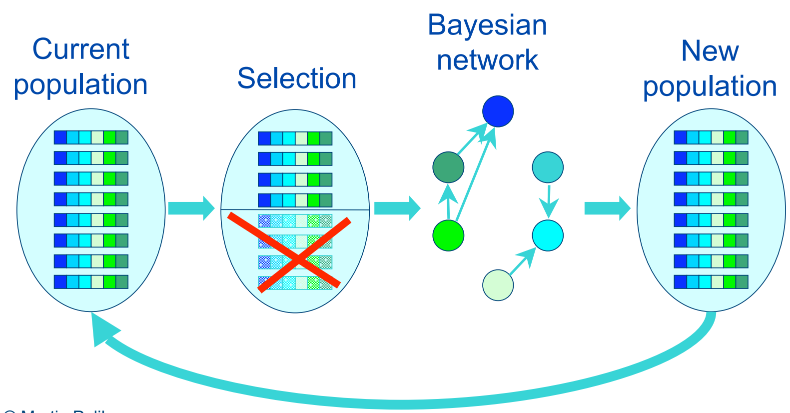
- Pelikan, Goldberg, & Cantú-Paz (1998)
- Use a Bayesian network (BN) as a model.
- Bayesian network
  - Acyclic directed graph.
  - Nodes are variables (string positions).
  - Conditional dependencies (edges).
  - Conditional independencies (implicit).

Example: Bayesian Network (BN)

- Conditional dependencies.
- Conditional independencies.



BOA



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

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

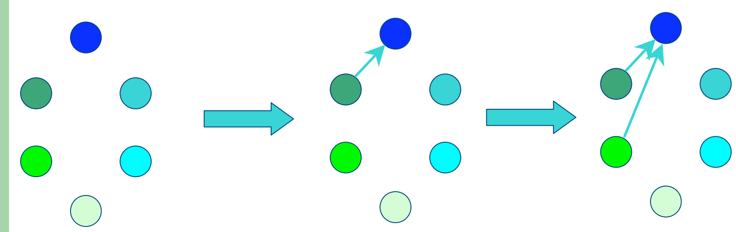
- Minimum description length metrics
  - Bayesian information criterion (BIC)

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

Learning BNs: Search Procedure

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

Learning BNs: Example



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

BOA Theory: Num. of Generations

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

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

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

$$O\left(n\right)$$

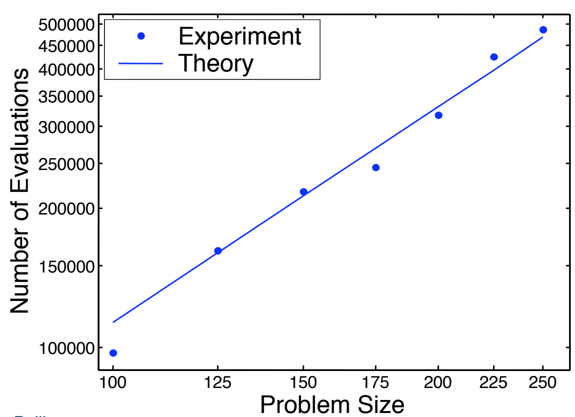
Good News: Challenge Met!

- Theory
  - Population sizing (Pelikan et al., 2000, 2002)
    1. Initial supply.
    2. Decision making.
    3. Drift.
    4. Model building.

    → O(n) to O($n^{1.05}$)
  - Iterations until convergence (Pelikan et al., 2000, 2002)
    1. Uniform scaling.
    2. Exponential scaling.

    → O($n^{0.5}$) to O(n)
- BOA solves order-k decomposable problems in O($n^{1.55}$) to O(n^2) evaluations!

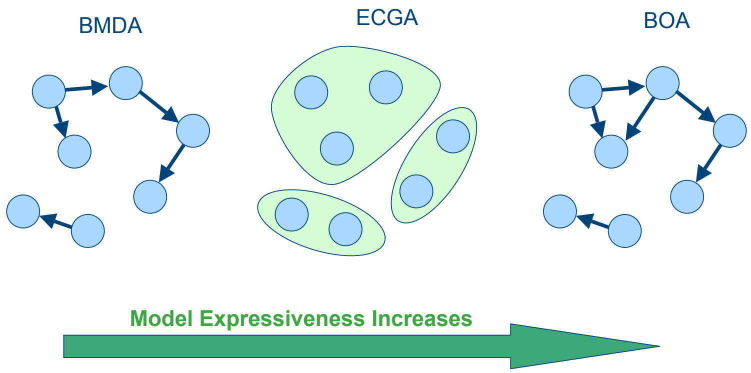
Theory vs. Experiment (5-bit Traps)



BOA Siblings

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

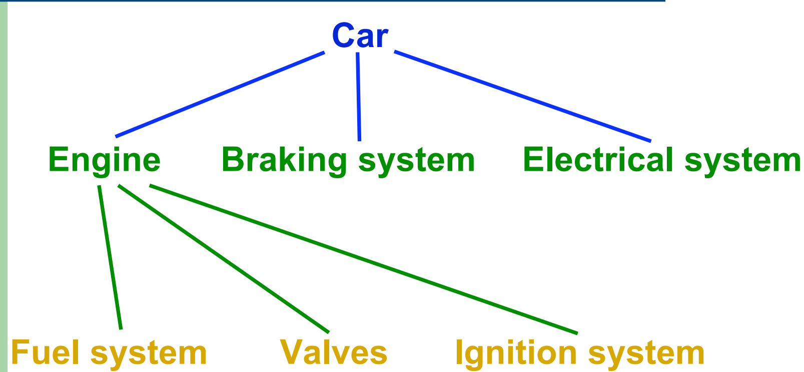
Model Comparison



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.

Hierarchical Decomposition



3 Keys to Hierarchy Success

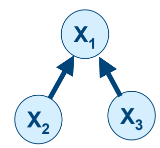
- Proper decomposition.
  - Must decompose problem on each level properly.
- Chunking.
  - Must represent & manipulate large order solutions.
- Preservation of alternative solutions.
  - Must preserve alternative partial solutions (chunks).

Hierarchical 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).

Local Structures in BNs

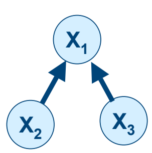
- Look at one conditional dependency.
  - 2^k probabilities for k parents.
- Why not use more powerful representations for conditional probabilities?

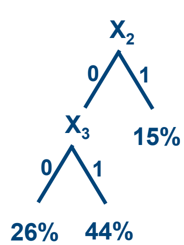


X_2X_3	$P(X_1=0 \mid X_2X_3)$
00	26 %
01	44 %
10	15 %
11	15 %

Local Structures in BNs

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





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*.

Efficiency Enhancement for PMBGAs

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

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 problem-specific knowledge

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)

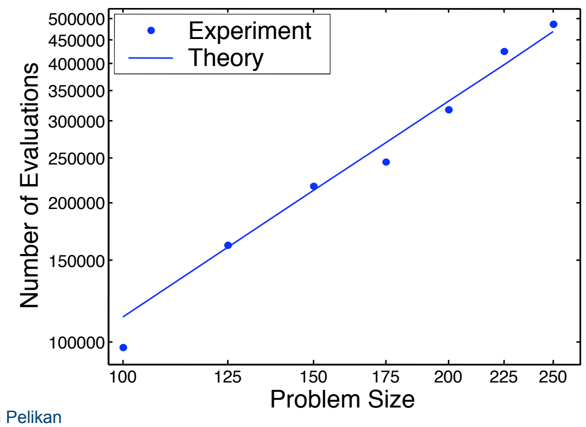
Promising Results with Discrete PMBGAs

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

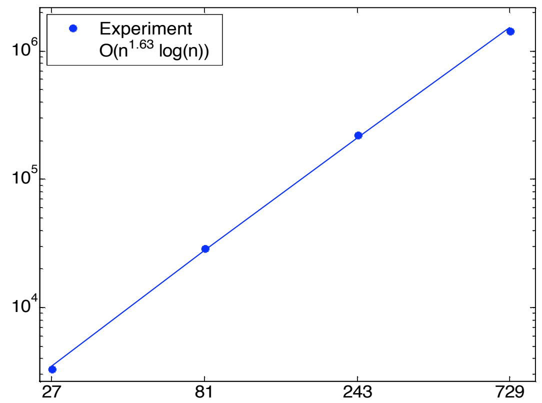
Results: Artificial Problems

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

BOA on Concatenated 5-bit Traps



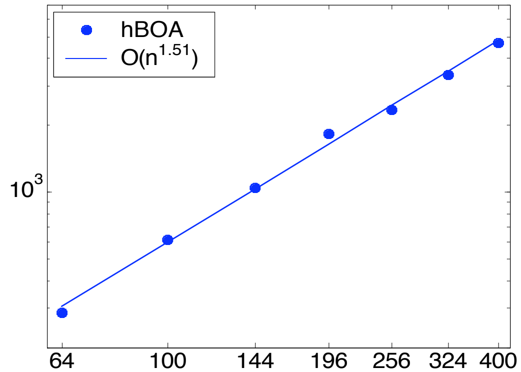
hBOA on Hierarchical Traps



Results: Physics

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

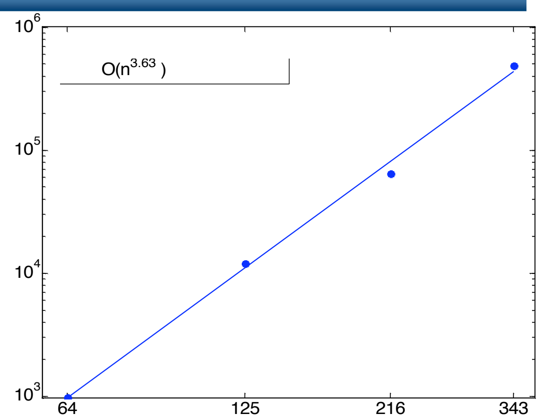
hBOA on Ising Spin Glasses (2D)



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 & Loebl, 1999)
- Great also on Gaussians.

hBOA on Ising Spin Glasses (3D)



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)

Results: 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)
- Quantum excitation chemistry (Sastry et al., 2005)

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

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.

Continuous PMBGAs

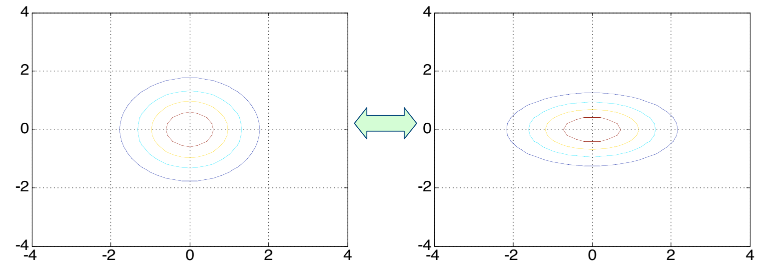
- New challenge
  - Infinite domain for each variable.
  - How to model?
- 2 approaches
  - Discretize and apply discrete model/PMBGA
  - Create continuous model
    - Estimate pdf.

PBIL Extensions: SHCwL

- 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.

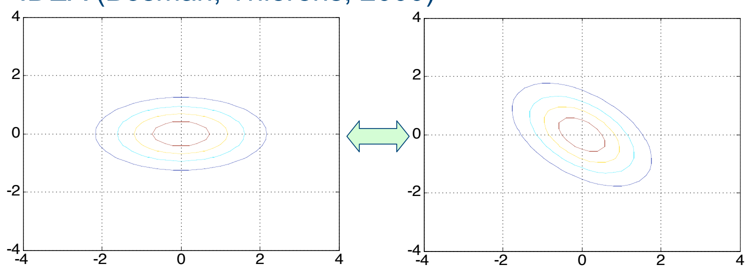
Use Different Deviations

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



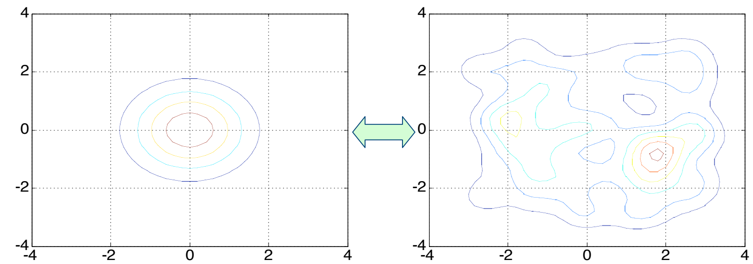
Use Covariance

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



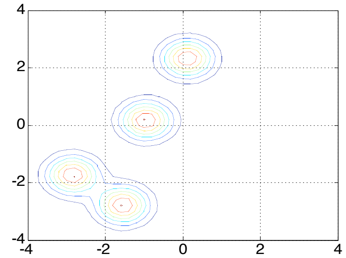
How Many Peaks?

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



Mixtures: Between One and Many

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



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.

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)

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

Continuous 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 2^k bins.
  - K-means clustering on each variable.
  - Pelikan, Goldberg, & Tsutsui (2003); Cantu-Paz (2001).

Continuous PMBGAs: Summary

- 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

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

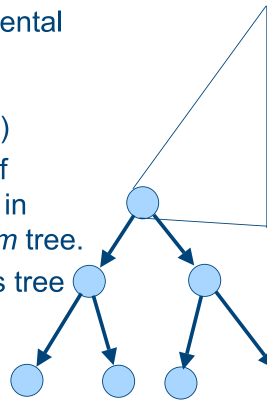
PMBGP (Genetic Programming)

- New challenge
  - Structured, variable length representation.
  - Possibly infinitely many values.
  - Position independence (or not)
- Approaches
  - Limit maximum complexity of a solution.
  - Allow complexity to change over time.

PIPE

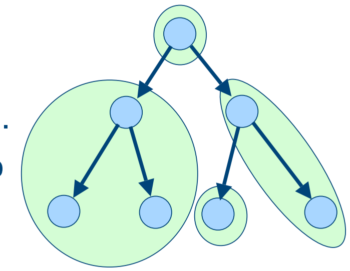
- Probabilistic incremental program evolution (Salustowicz & Schmidhuber, 1997)
- Store frequencies of operators/terminals in nodes of a *maximum* tree.
- Sampling generates tree from top to bottom

X	P(X)
sin	0.15
+	0.35
-	0.35
X	0.15



eCGP

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



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.

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

PMBGAs for Permutations

- New challenges
  - Relative order
  - Absolute order
  - Permutation constraints
- Two basic approaches
  - Random-key representation with real-valued PMBGAs
  - Probabilistic models for permutations

Random Keys and PMBGAs

- 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)

Direct Modeling of Permutations

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

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 (again).

Starting Points

- WWW
  - Laboratory home pages.
  - Authors' home pages.
  - Research index (www.researchindex.com)
  - Google (www.google.com)
  - Google scholar (scholar.google.com)
- Introductory material
  - Pelikan et al. (2002). A survey to optimization by building and using probabilistic models. Computational optimization and applications, 21(1)
  - Larrañaga & Lozano (editors) (2001). Estimation of distribution algorithms: A new tool for evolutionary computation. Kluwer.

Code

- 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`