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.

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.

Probabilistic Model-Building Genetic Algorithms

a.k.a. Estimation of Distribution Algorithms

a.k.a. Iterated Density Estimation Algorithms

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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.

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 + their evaluation:

<table>
<thead>
<tr>
<th>#</th>
<th>Solution</th>
<th>Evaluation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>00100</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>11011</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>01101</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>10111</td>
<td>3</td>
</tr>
</tbody>
</table>

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**

Current population → Selected population → Probabilistic Model → New population

...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 \( \mathbf{p} = (p_1, \ldots, p_n) \)
  - \( p_i \) = 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), (Baluja, 1994)

<table>
<thead>
<tr>
<th>Current population</th>
<th>Selected population</th>
<th>New population</th>
</tr>
</thead>
<tbody>
<tr>
<td>11001</td>
<td>11001</td>
<td>11101</td>
</tr>
<tr>
<td>10101</td>
<td>10101</td>
<td>11001</td>
</tr>
<tr>
<td>01011</td>
<td>11000</td>
<td>10101</td>
</tr>
</tbody>
</table>

Probability vector: 1.0 0.5 0.5 0.0 1.0

**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.

**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: 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.
  - 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

Trap-5

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 \( p(00000), p(00001), \ldots, p(11111) \)
- Sample model
  - Sample 5 bits at a time
  - Generate 00000 with \( p(00000) \), 00001 with \( p(00001) \), ...

---

Correct Model on Traps: Dynamics

- 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 xover: \( O(2^n) \) (w/o tight linkage).

---

Good News: Good Stats Work Great!
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)

<table>
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<tr>
<th>Model</th>
<th>$P(X=1)$</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>75%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>String</th>
</tr>
</thead>
</table>

| $X$ | $P(Y=1|X)$ |
|-----|------------|
| 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.
  - 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: $O(n^2)$

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:
  \[
  \text{MDL}(M,D) = D_{\text{Model}} + D_{\text{Data}}
  \]
- Each frequency needs \((0.5 \log N)\) bits:
  \[
  D_{\text{Model}} = \sum_{g \in G} 2^{\log \frac{1}{g}} \log N
  \]
- Each solution \(X\) needs \(-\log p(X)\) bits:
  \[
  D_{\text{Data}} = -N \sum_X p(X) \log p(X)
  \]

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 \(O(\sqrt{k \log n})\) times faster than ECGA!
  - But only for separable problems (and similar ones).

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.
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.

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

- **Minimum description length metrics**
  - Bayesian information criterion (BIC)
    \[
    BIC(B) = \sum_{i=1}^{n} \left( -H(X_i | \Pi_i)N + 2 \log \frac{N}{2} \right)
    \]

### 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.
  \[
  O(2^1)
  \]

- Decision making (Harik et al, 1997)
  - Decide well between competing partial sols.
  \[
  O(\sqrt{n \log n})
  \]

- Drift (Thierens, Goldberg, Pereira, 1998)
  - Don’t lose less salient stuff prematurely.
  \[
  O(n)
  \]

- Model building (Pelikan et al., 2000, 2002)
  - Find a good model.
  \[
  O(n^{1.05})
  \]

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

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

Another Option: Markov Networks

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

Model Comparison

- BMDA
- ECGA
- BOA

.Model Expressiveness Increases

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.
Hierarchical Decomposition

- Car
  - Engine
  - Braking system
  - Electrical system
  - Fuel system
  - Valves
  - Ignition system

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 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 %              |
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 $y$.

Hierarchical Traps: The Ultimate Test

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

hBOA on Hierarchical Traps

- Graph showing the relationship between problem size and number of evaluations.
- Experiment data follows the trend $O(n^{1.63} \log(n))$. 

GECCO 2007 Tutorial / Probabilistic Model-Building Genetic Algorithms
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

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

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

<table>
<thead>
<tr>
<th>Problem Size</th>
<th>Number of Evaluations</th>
</tr>
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<tbody>
<tr>
<td>250</td>
<td>100000</td>
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<tr>
<td>255</td>
<td>125000</td>
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<td>260</td>
<td>200000</td>
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<td>265</td>
<td>300000</td>
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<td>270</td>
<td>400000</td>
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hBOA on Hierarchical Traps

<table>
<thead>
<tr>
<th>Problem Size</th>
<th>Number of Evaluations</th>
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<tbody>
<tr>
<td>27</td>
<td>10</td>
</tr>
<tr>
<td>81</td>
<td>100</td>
</tr>
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<td>243</td>
<td>4</td>
</tr>
<tr>
<td>729</td>
<td>10</td>
</tr>
</tbody>
</table>

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)

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)

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: 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)
- Minimum vertex cover (Pelikan et al., 2007)

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: 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 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.
  - 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)

- 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.
  - 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

- 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).
  - 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

<table>
<thead>
<tr>
<th>X</th>
<th>P(X)</th>
</tr>
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<tbody>
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</tr>
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<td>-</td>
<td>0.35</td>
</tr>
<tr>
<td>X</td>
<td>0.15</td>
</tr>
</tbody>
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**BOA for GP**

- 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.

**eCGP**

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

**MOSES**

- 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.
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)

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 and real-valued PMBGAs
  - Explicit probabilistic models for permutations

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 $A=(a_{i,j})_{i,j=1, 2, ..., n}$
  - $a_{i,j}$ 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
Code

- BOA, BOA with decision graphs, dependency-tree EDA
  [http://medal.cs.umsl.edu/](http://medal.cs.umsl.edu/)
- ECGA, BOA, and BOA with decision trees/graphs
  [http://www-illigal.ge.uiuc.edu/](http://www-illigal.ge.uiuc.edu/)
- mBOA
- PIPE
  [http://www.idsia.ch/~rafal/](http://www.idsia.ch/~rafal/)
- Real-coded BOA
- Demos of APS and EHBSA
  [http://www.hannan-u.ac.jp/~tsutsui/research-e.html](http://www.hannan-u.ac.jp/~tsutsui/research-e.html)