Estimation of Distribution Algorithms

EVO Lecture 13

Simon Poulding

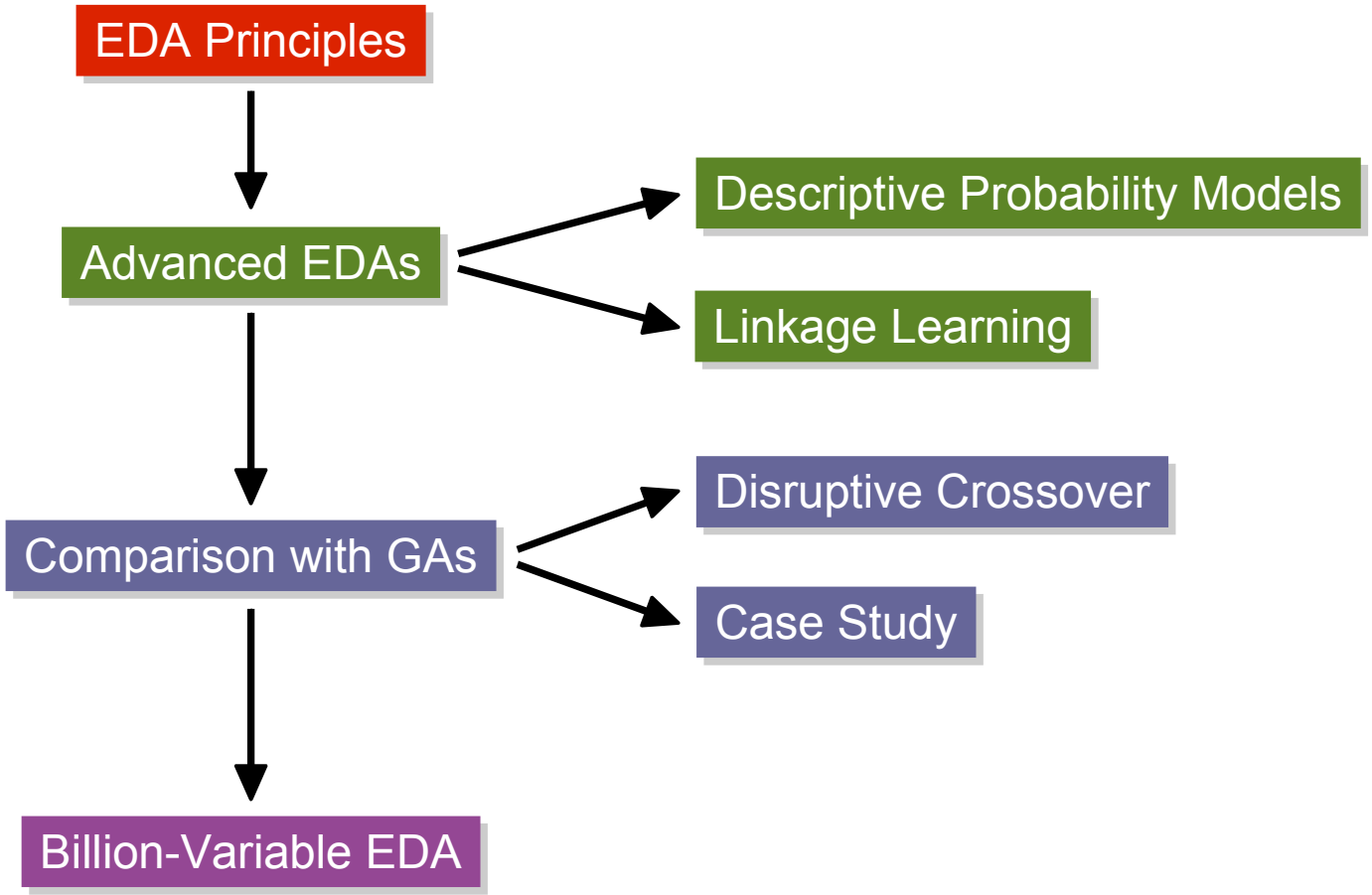
December 2010

Motivation

Estimation of Distribution Algorithms (EDAs)
Probabilistic Model-Building Genetic Algorithms (PMBGAs)
Iterated Density-Estimation Evolutionary Algorithms (IDEAs)

- modern form of evolutionary algorithm
- solve problem classes where standard GAs fail
- trajectories

Road Map


EDA Principles
Advanced EDAs
Descriptive Probability Models
Linkage Learning
Comparison with GAs
Disruptive Crossover
Case Study
Billion-Variable EDA

Quick Review of Probability I

Probability

- 7 random observations of my state of mind
- if X is a random variable representing my state of mind, can estimate its distribution as:

$$\mathbb{P}(X = \text{happy}) = \frac{4}{7}$$

$$\mathbb{P}(X = \text{sad}) = \frac{3}{7}$$

State
sad
sad
happy
happy
sad
happy
happy

Quick Review of Probability II

Conditional Probability

- if D is the day,

$$\mathbb{P}(X = \text{happy} | D = \text{Monday}) = \frac{1}{3}$$

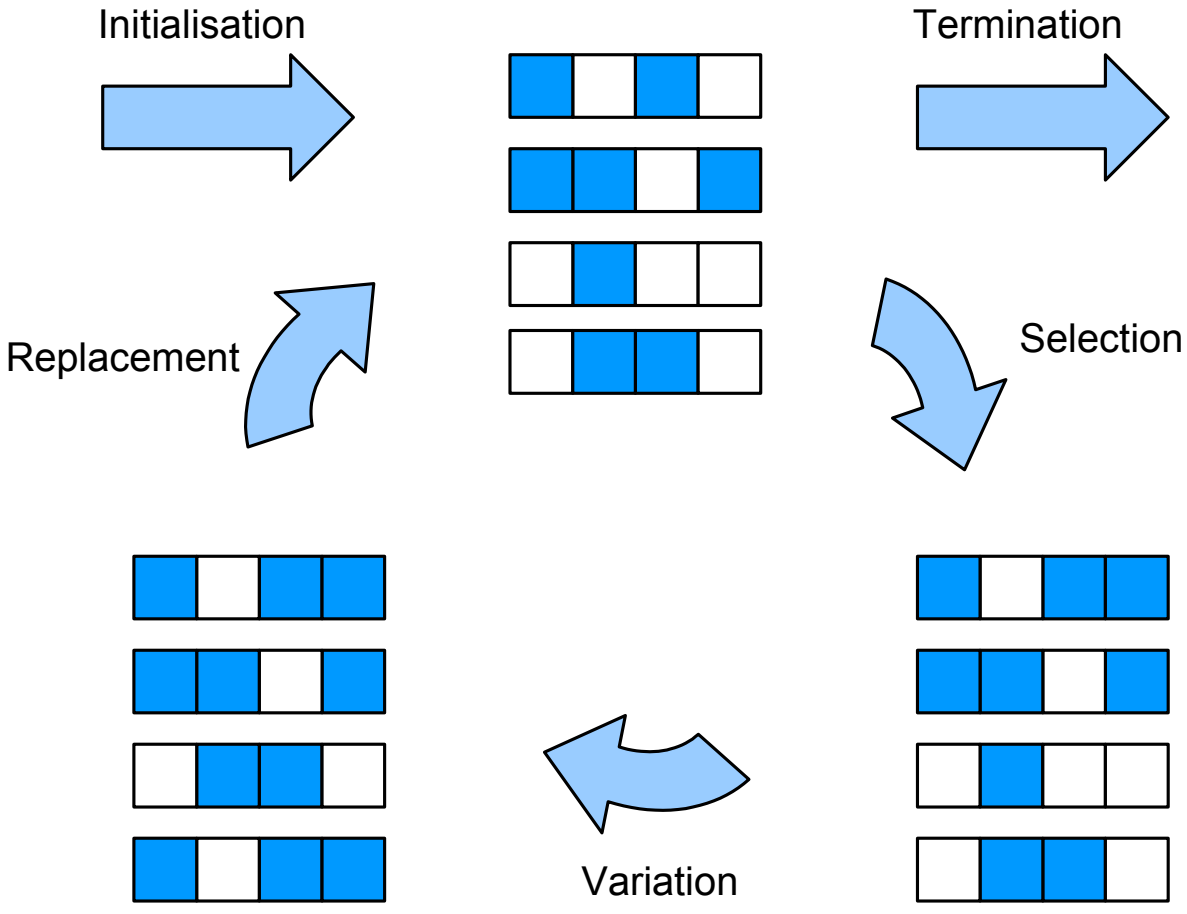
$$\mathbb{P}(X = \text{sad} | D = \text{Monday}) = \frac{2}{3}$$

- enables a more 'refined' model
- conditional probability can be calculated using:

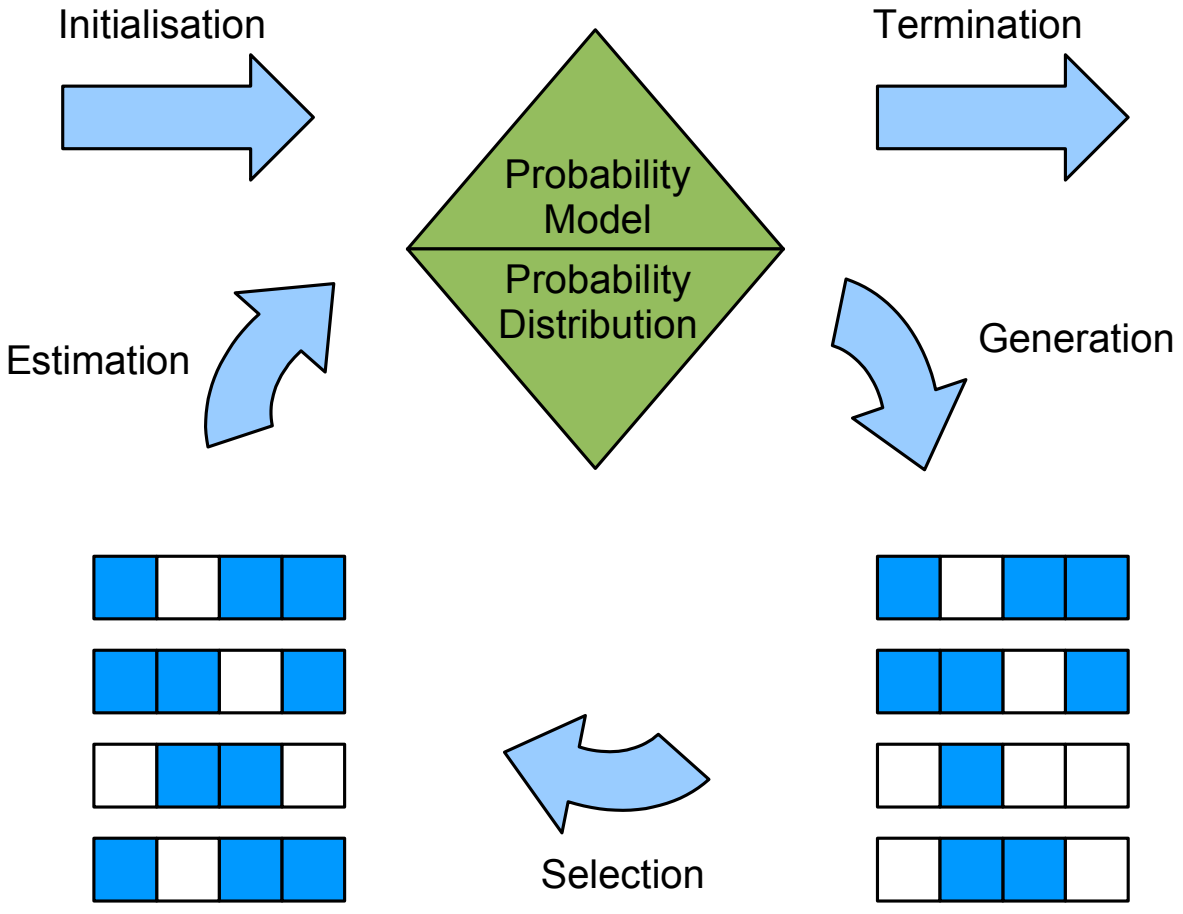
$$\mathbb{P}(X = x | D = d) = \frac{\mathbb{P}(X = x, D = d)}{\mathbb{P}(D = d)}$$

Day	State
Monday	sad
Monday	sad
Monday	happy
Friday	happy
Friday	sad
Friday	happy
Friday	happy

Genetic Algorithm Process



Estimation of Distribution Algorithm Process



A Simple Example - Configuration

Genome (Representation)

4 genes (X_i, $i = 0, 1, 2, 3$); each gene is either A or B

Probability Model

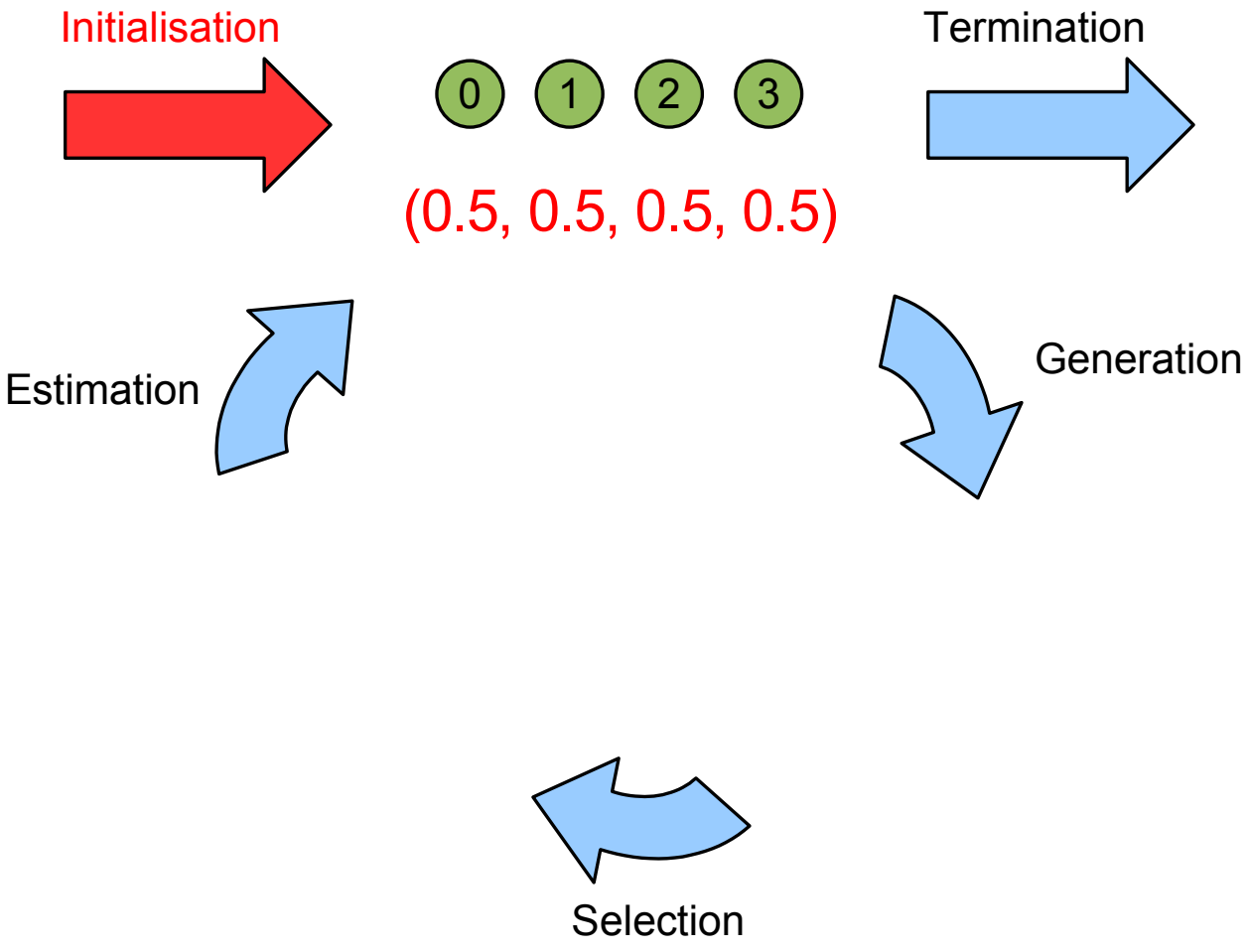
assume each gene is independent

Probability Distribution

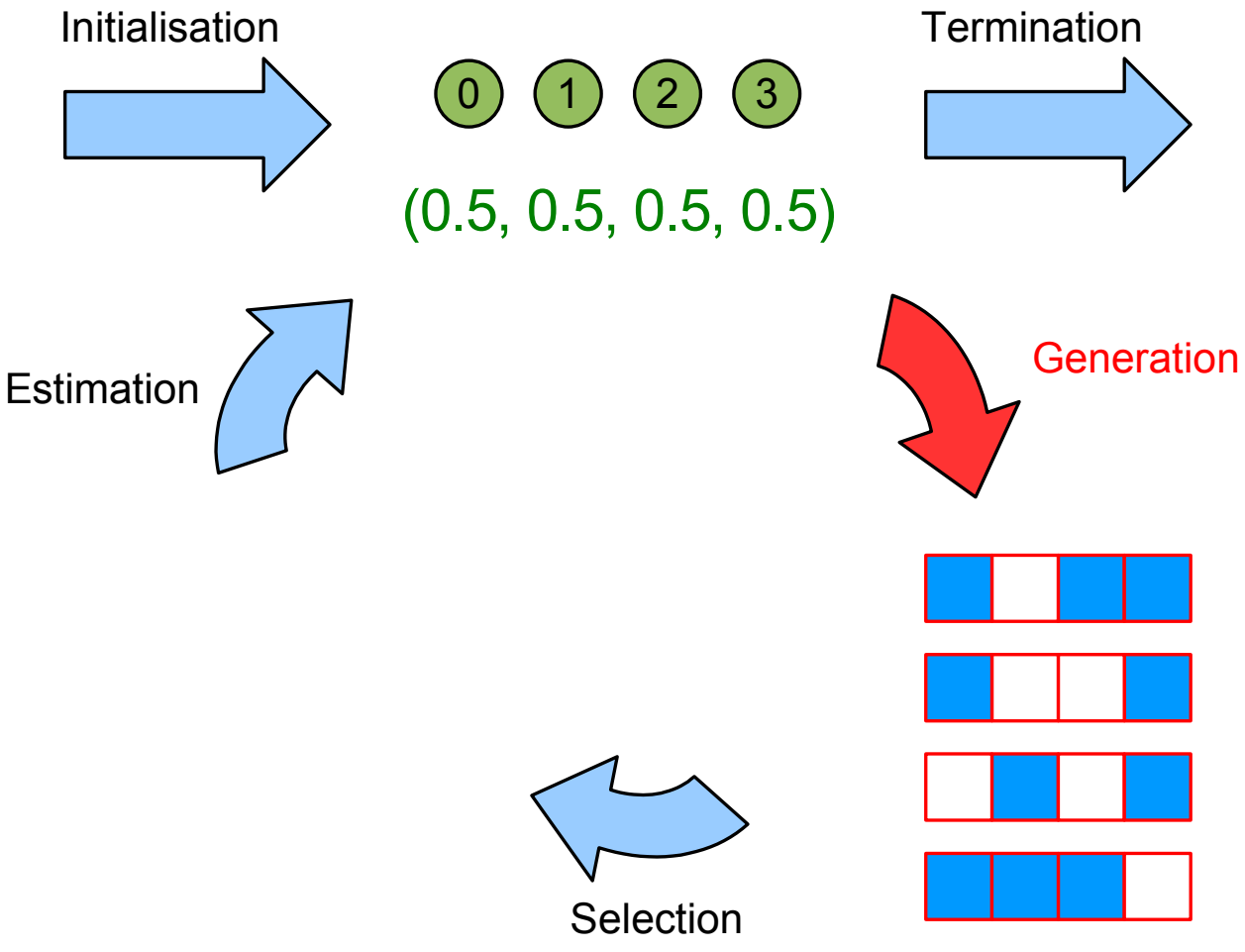
$$(p_0, p_1, p_2, p_3)$$

where $\mathbb{P}(X_i = \mathrm{A}) = p_i$ and thus $\mathbb{P}(X_i = \mathrm{B}) = 1 - p_i$

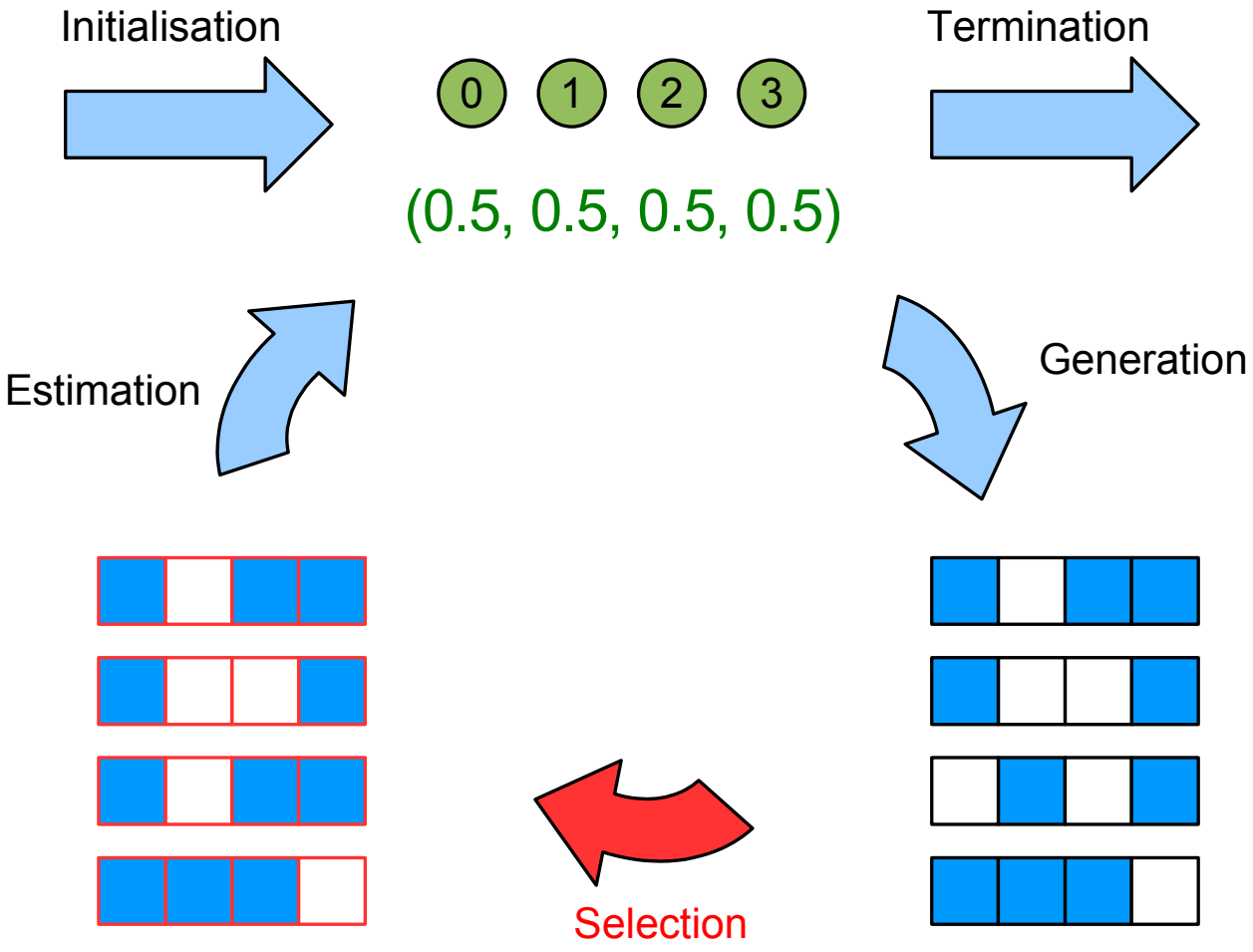
A Simple Example - Process



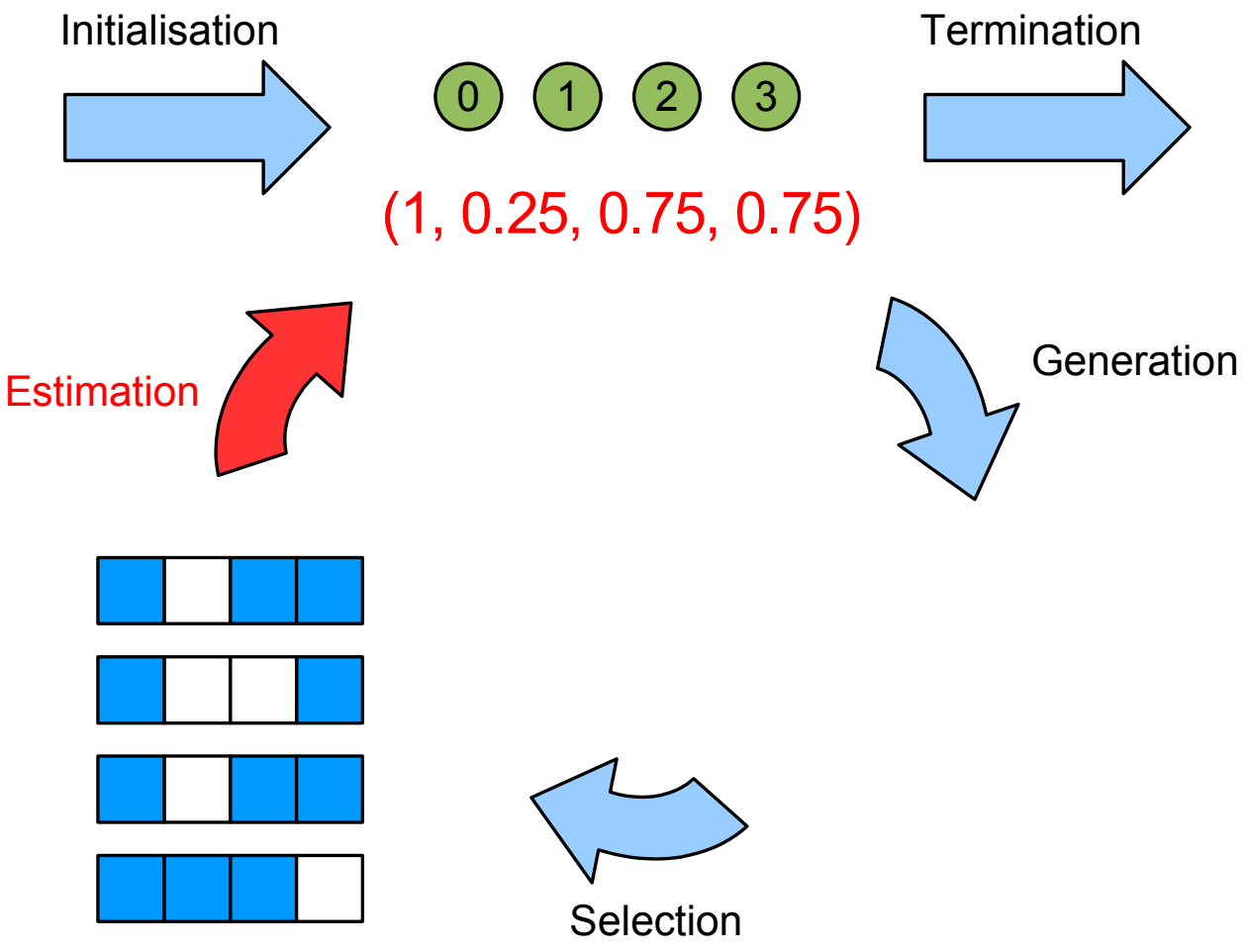
A Simple Example - Process



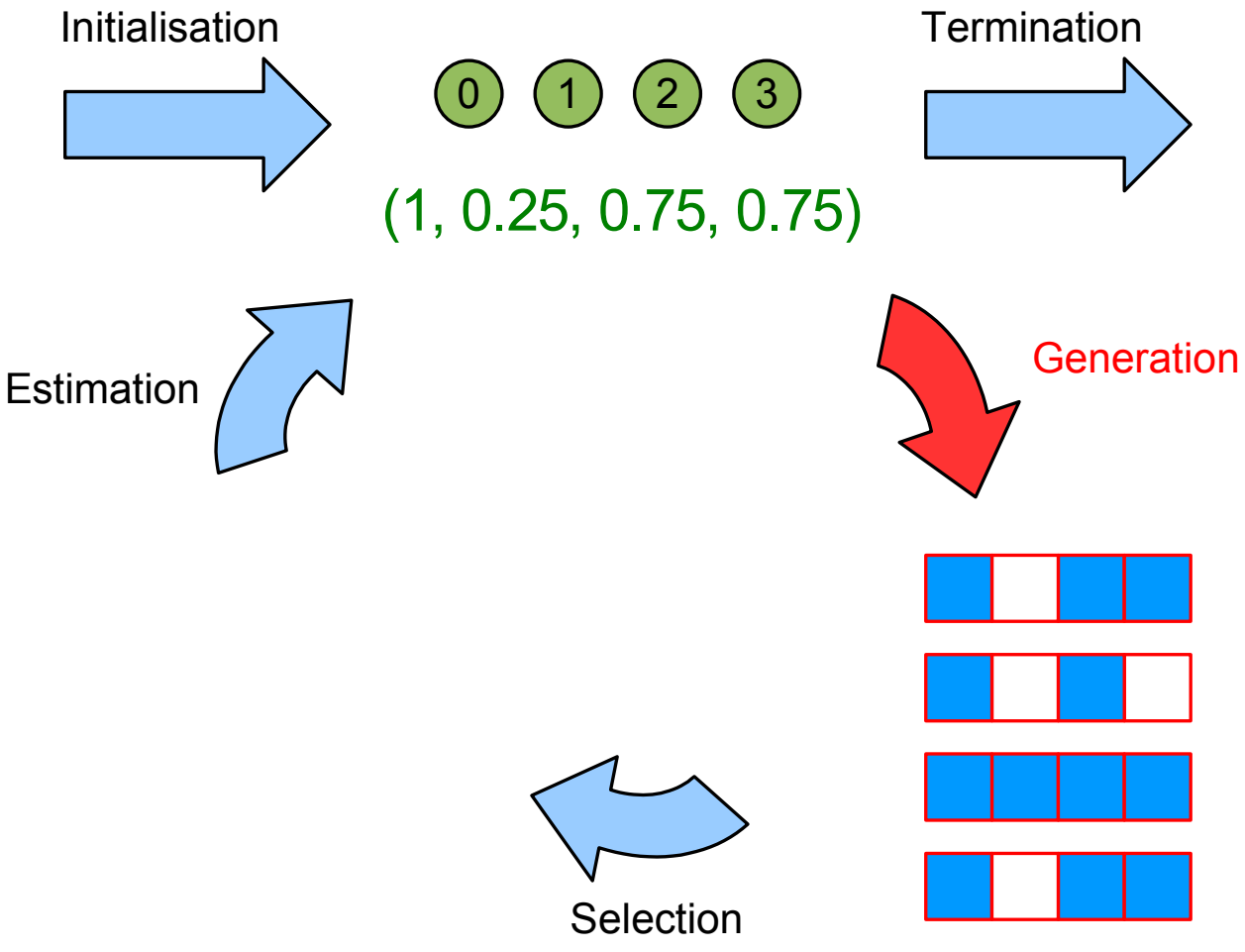
A Simple Example - Process



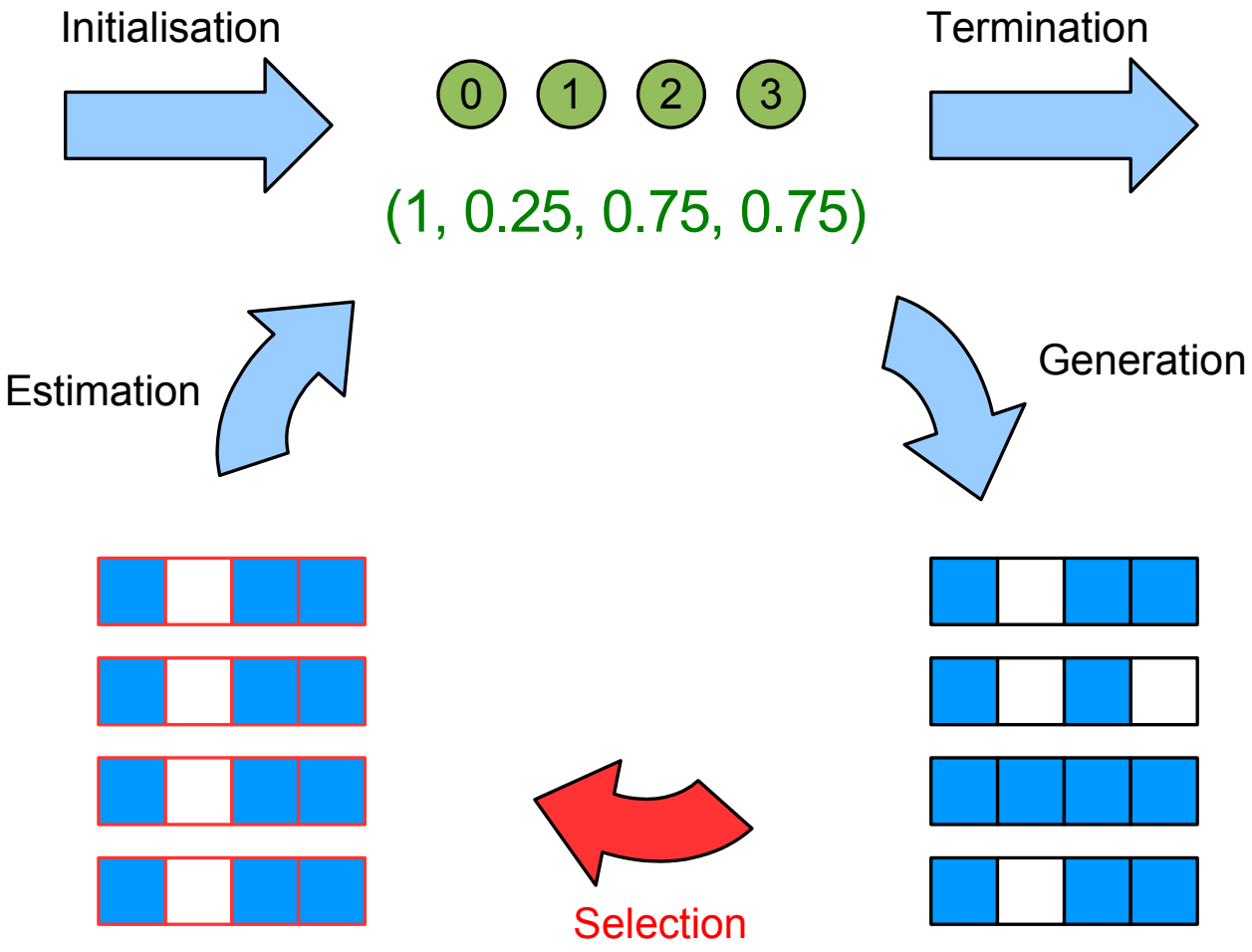
A Simple Example - Process



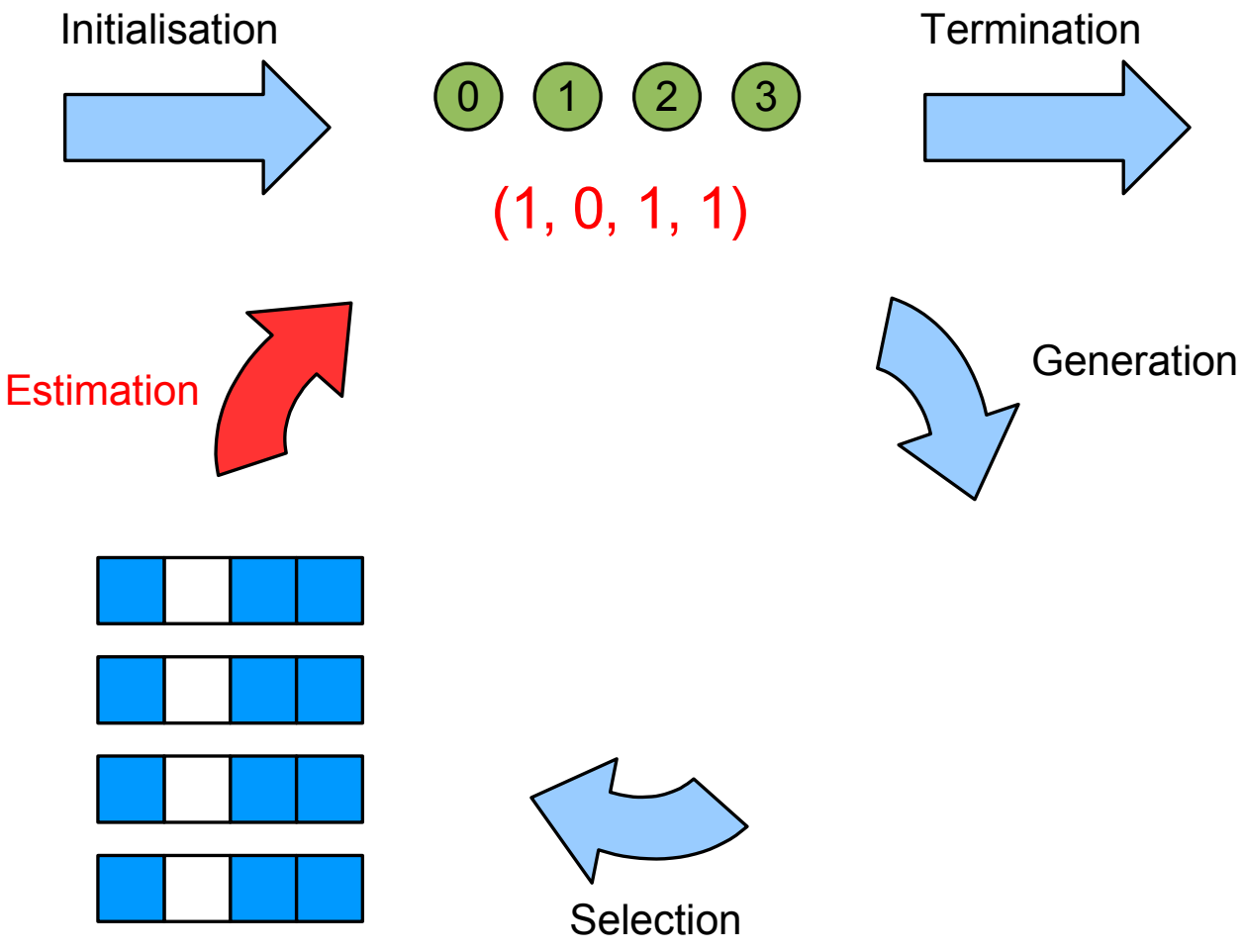
A Simple Example - Process



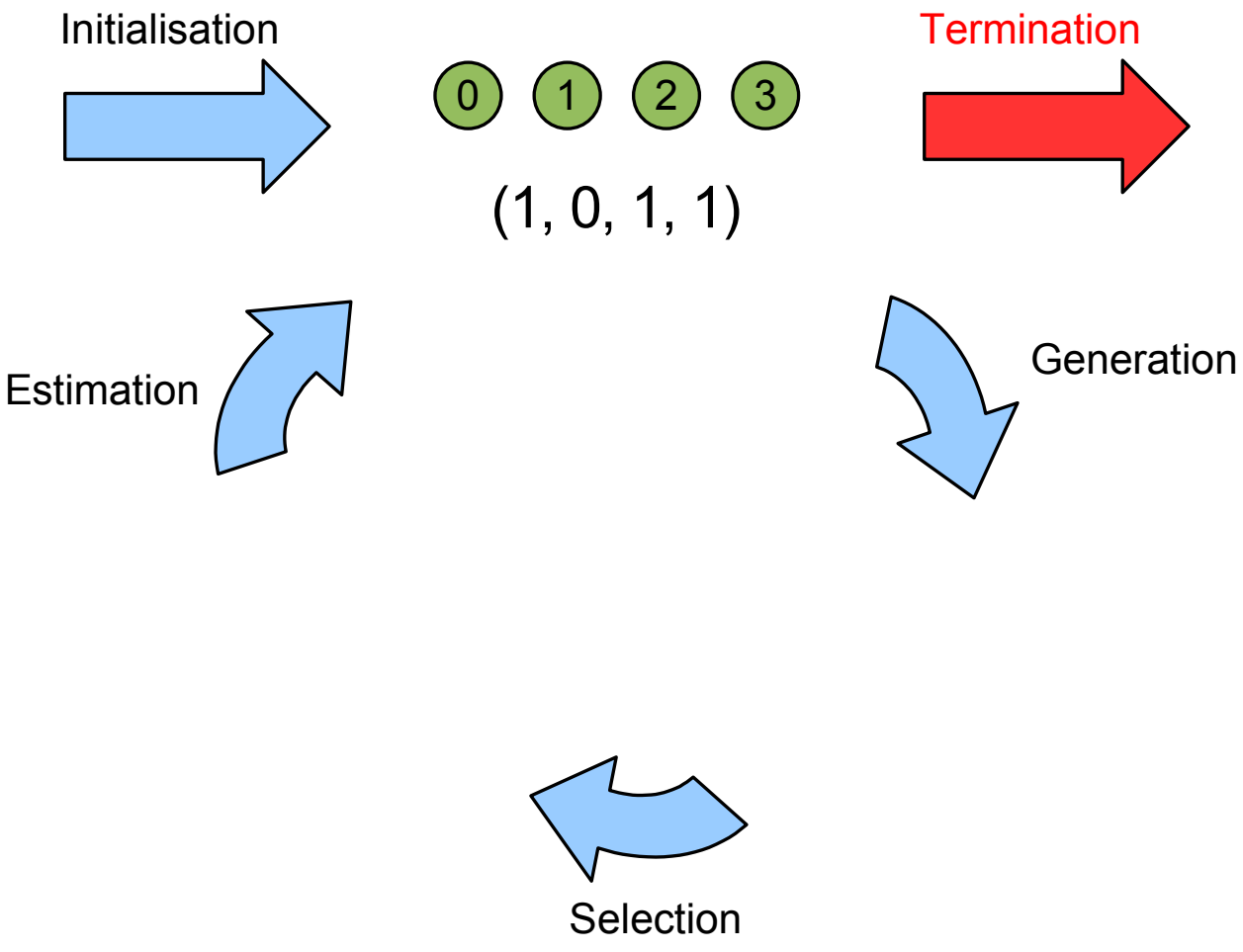
A Simple Example - Process



A Simple Example - Process



A Simple Example - Process



A Simple Example - Key Points I

Initialisation

Initially, don't know distributions of A and B in best solutions, so assume equally likely: $p_i = 0.5$.

Generation

Could use the following method to pick the value of each gene, X_i:

1. pick a (uniformly distributed) random number, γ, between 0 and 1
2. if $\gamma \leq p_i$, then set X_i to A, otherwise to B

Note: The values in the generated population will match the distribution closely, but not necessarily exactly.

A Simple Example - Key Points II

Selection

Can use same selection methods as for standard GAs, e.g. proportional selection (roulette wheel).

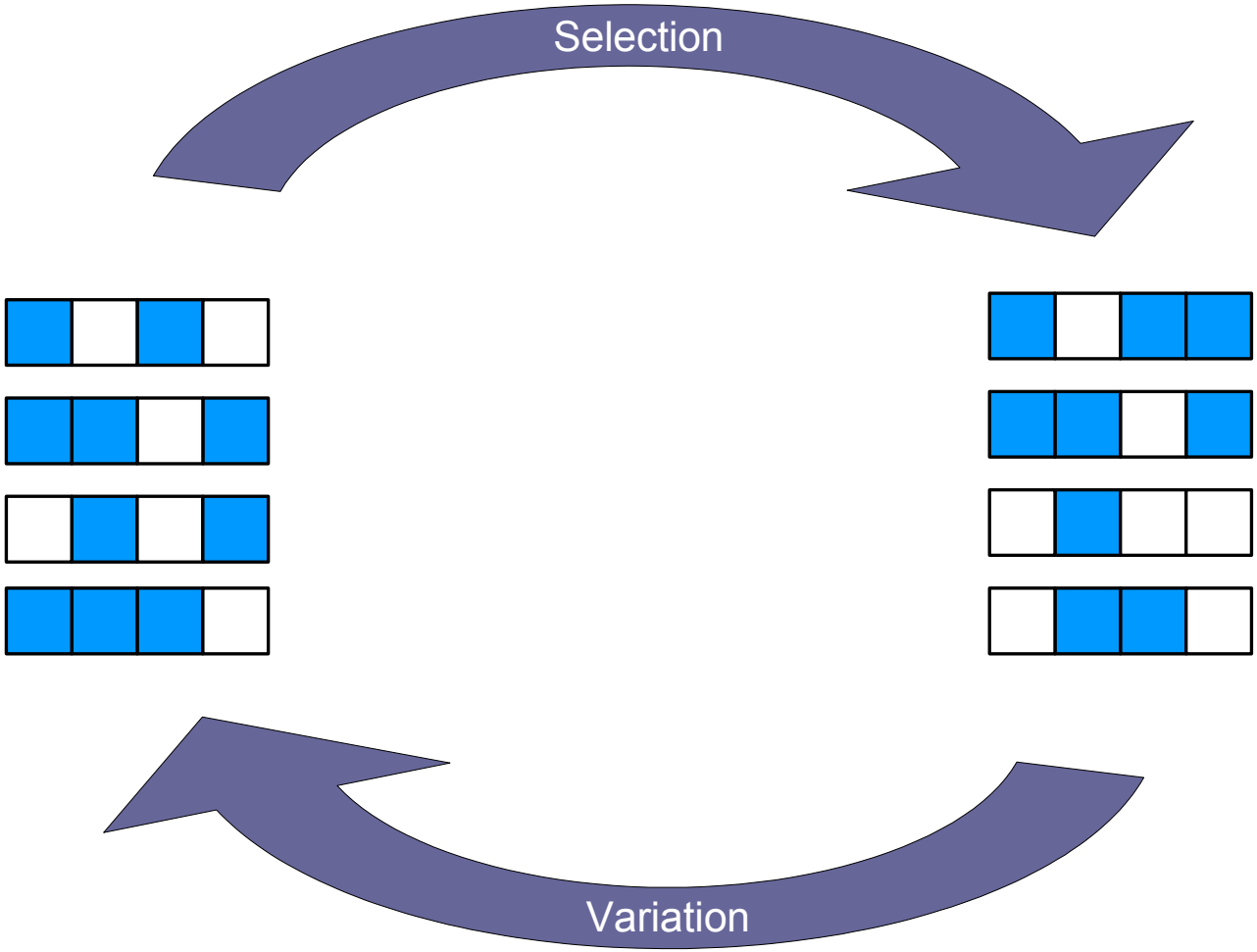
Estimation

In this example, simply count the number of As for gene X_i and divide by the number of individuals to give p_i.

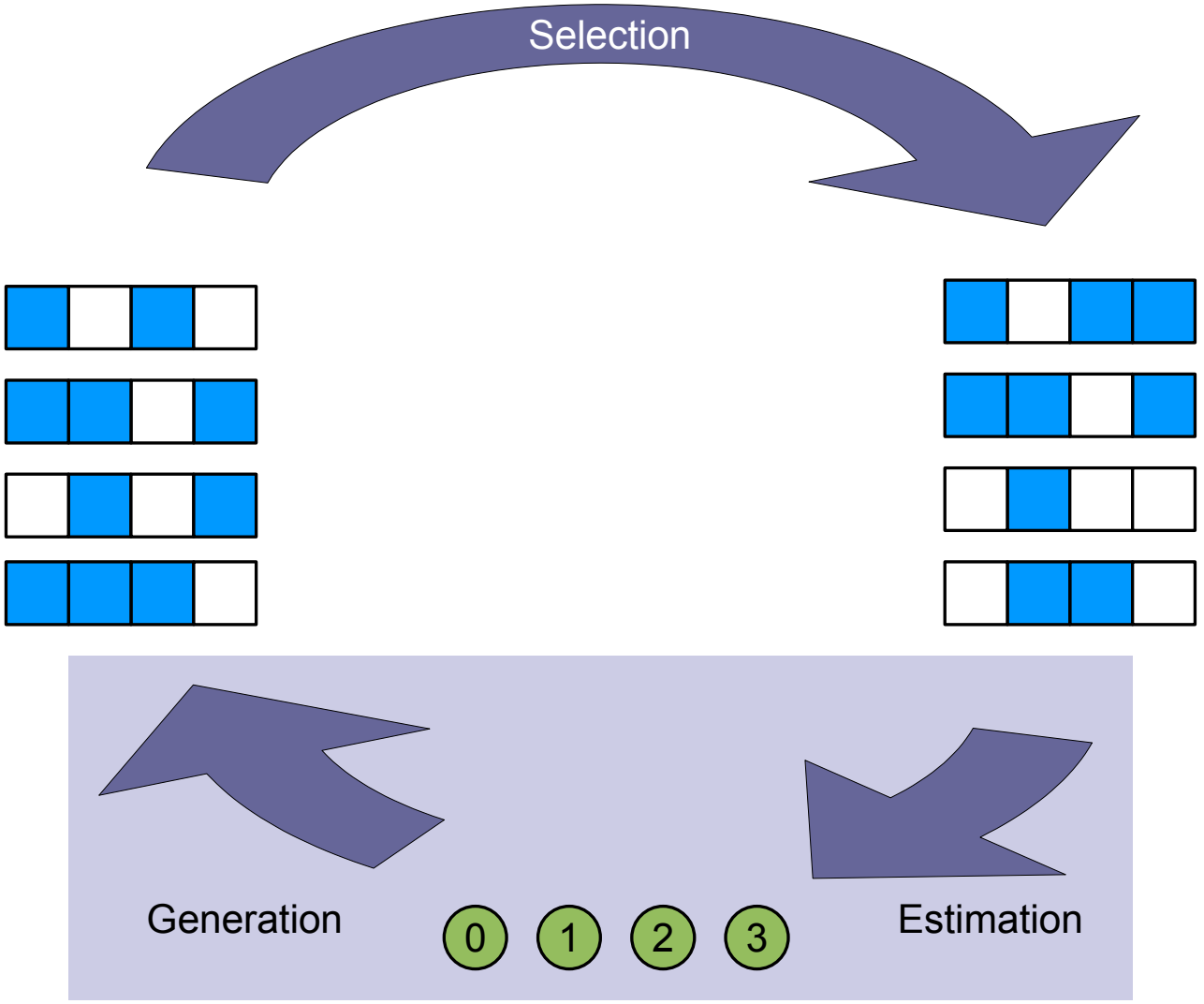
Termination

Sensible criterion is for all p_i to be either 0 or 1.
Note: The solution is ABAA; it is *not* (1,0,1,1). The latter is the *probability distribution* at termination.

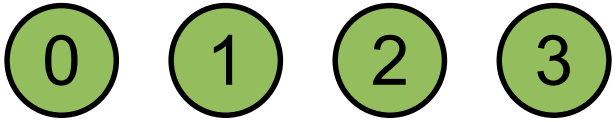
EDAs as GAs with Variance Operator



EDAs as GAs with Variance Operator



Univariate Probability Models



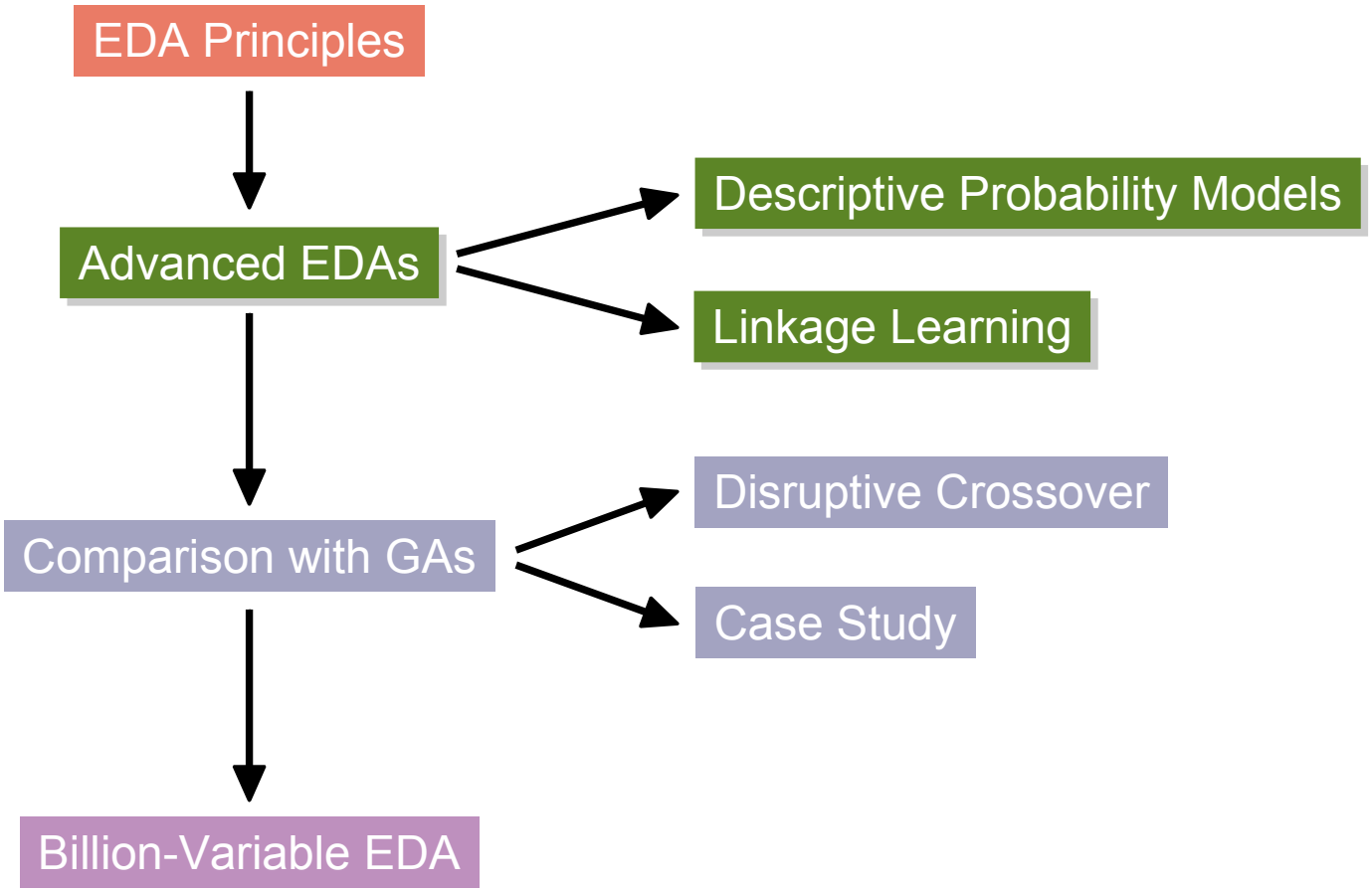
This model is used by the following EDAs (although the algorithm itself differs slightly):

- Univariate Marginal Distribution Algorithm (UMDA) [Mühlenbein and Paaß, 1996]
- Population-Based Incremental Learning (PBIL) [Baluja, 1994]
- Compact Genetic Algorithm (cGA) [Harik *et al.*, 1999]

But ...

Is the assumption of independent probability distributions for each gene an oversimplification?

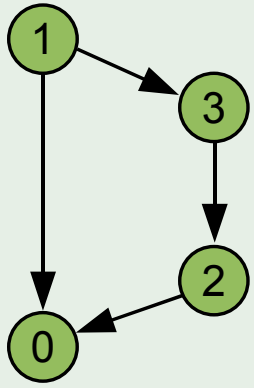
Road Map


EDA Principles
Advanced EDAs
Descriptive Probability Models
Linkage Learning
Comparison with GAs
Disruptive Crossover
Case Study
Billion-Variable EDA

Conditional Probability Models

Probability distribution for a gene depends on (conditional on) the value of other genes.

Example



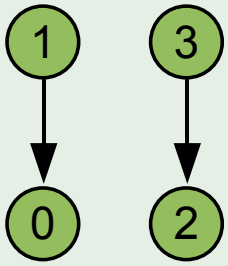
- distribution of X_1 is independent (as before)
- but, distribution of X_3 depends on value of X_1
- distribution of X_2 depends on value of X_3
- distribution of X_0 depends on values of X_1 *and* X_2

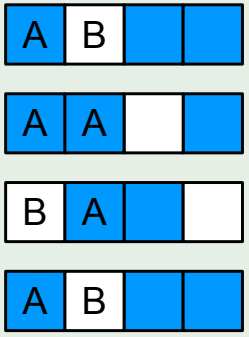
(arrows go from parent(s) to dependent child)

Need to order genes appropriately in order to generate from, and estimate, the distribution.

Conditional Probability Model Calculations I

Estimation Example





$\mathbb{P}(X_1 = \mathrm{A}) = 0.5$ and so $\mathbb{P}(X_1 = \mathrm{B}) = 0.5$

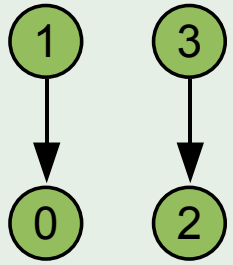
$\mathbb{P}(X_0 = \mathrm{A} | X_1 = \mathrm{A}) = 0.5$ and so $\mathbb{P}(X_0 = \mathrm{B} | X_1 = \mathrm{A}) = 0.5$

$\mathbb{P}(X_0 = \mathrm{A} | X_1 = \mathrm{B}) = 1$ and so $\mathbb{P}(X_0 = \mathrm{B} | X_1 = \mathrm{B}) = 0$

Conditional Probability Model Calculations II

Generation Example

- $\mathbb{P}(X_1 = \mathrm{A}) = 0.5$
- $\mathbb{P}(X_0 = \mathrm{A} | X_1 = \mathrm{A}) = 0.5$
- $\mathbb{P}(X_0 = \mathrm{A} | X_1 = \mathrm{B}) = 1$



1. randomly pick γ_1 between 0 and 1, say $\gamma_1 = 0.428\ldots$
2. since $\gamma_1 \leq \mathbb{P}(X_1 = \mathrm{A})$, set X_1 to A
3. now pick γ_0 between 0 and 1, say $\gamma_0 = 0.732\ldots$
4. since $\gamma_0 > \mathbb{P}(X_0 = \mathrm{A} | X_1 = \mathrm{A})$, set X_0 to B
5. so in our generated individual, $X_0 = \mathrm{B}$, $X_1 = \mathrm{A}$

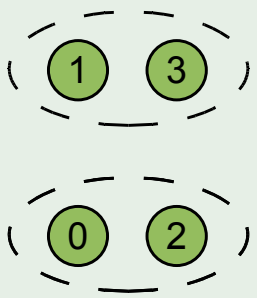
Subset Probability Models

Probability distributions considered for a subset of genes taken as a whole.

Example

for each subset, need to store probability of all combinations, e.g.:

$$\mathbb{P}(X_1 = \mathrm{A}, X_3 = \mathrm{A})$$
$$\mathbb{P}(X_1 = \mathrm{A}, X_3 = \mathrm{B})$$
$$\mathbb{P}(X_1 = \mathrm{B}, X_3 = \mathrm{A})$$
$$\mathbb{P}(X_1 = \mathrm{B}, X_3 = \mathrm{B})$$



Why Use More Complex Models?

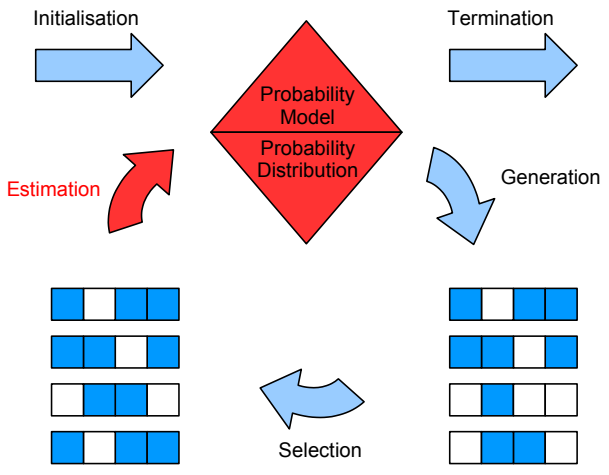
- Better able to model structure of underlying problem in terms of the relationship between genes
- Processing for estimating and generating from a more complex model is not usually significant compared to fitness evaluation
- Factorised Distribution Algorithm (FDA) [Mühlenbein, Mahning, and Rodriguez, 1998] uses a predefined model using conditional probability and subsets

But ...

Is is realistic that we define structure of probability model for problems in general?

Linkage (Model) Learning

- So far, examples have used a predefined probability model that stays the same throughout the algorithm
- Many powerful EDAs 'learn' the probability model at they go
- Often the probability model is derived during the estimation step of each generation

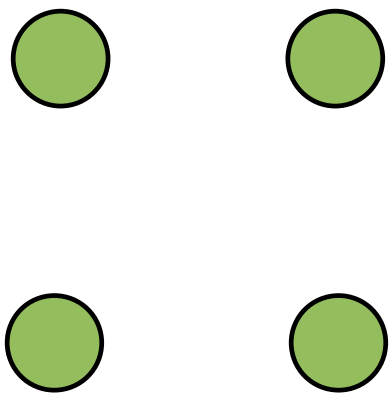


Model Metrics

- To be able to choose from all possible models, need to have a measure of how good a particular model is at representing the selected population
- Examples of metrics include:
  - Bayesian Dirichlet metric
  - Kullback-Leibler divergence
  - Pearson's chi-square statistic
  - minimum description length

Deriving the Model

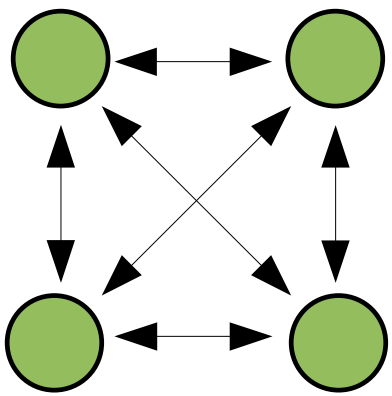
Given a metric, a possible method of deriving the model from the selected population is the following greedy algorithm:



1. assume no connections (all genes independent)

Deriving the Model

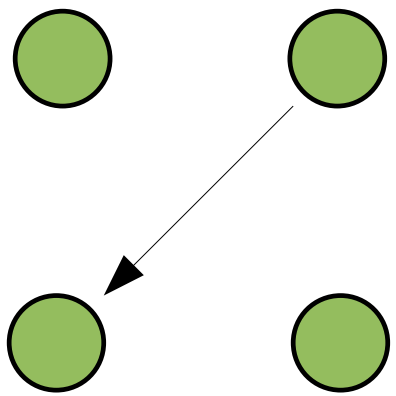
Given a metric, a possible method of deriving the model from the selected population is the following greedy algorithm:



1. assume no connections (all genes independent)
2. consider all valid operations on the model (e.g. adding a link from a parent to a child)

Deriving the Model

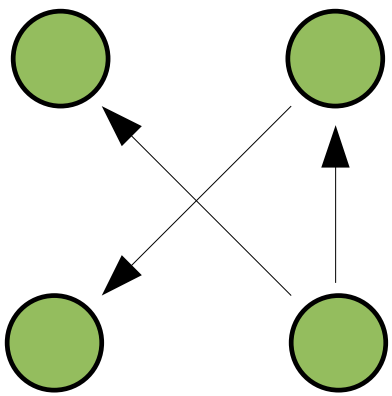
Given a metric, a possible method of deriving the model from the selected population is the following greedy algorithm:



1. assume no connections (all genes independent)
2. consider all valid operations on the model (e.g. adding a link from a parent to a child)
3. if no operation improves the metric, stop
4. otherwise perform the operation that improves the metric the most

Deriving the Model

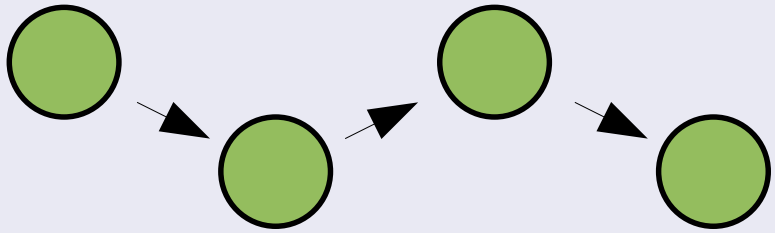
Given a metric, a possible method of deriving the model from the selected population is the following greedy algorithm:



1. assume no connections (all genes independent)
2. consider all valid operations on the model (e.g. adding a link from a parent to a child)
3. if no operation improves the metric, stop
4. otherwise perform the operation that improves the metric the most
5. repeat from step (2)

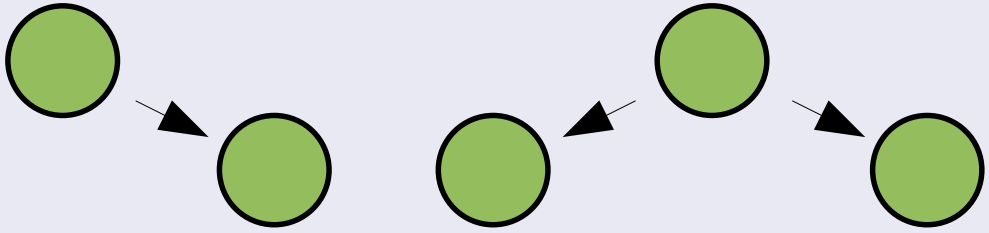
Examples of Linkage Learning EDAs I

Mutual Information Maximizing Input Clustering (MIMIC)



De Bonet *et al.*, 1997

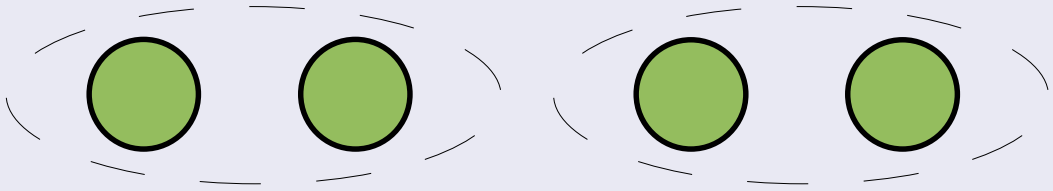
Bivariate Marginal Distribution Algorithm (BMDA)



Pelikan and Mühlenbein, 1999

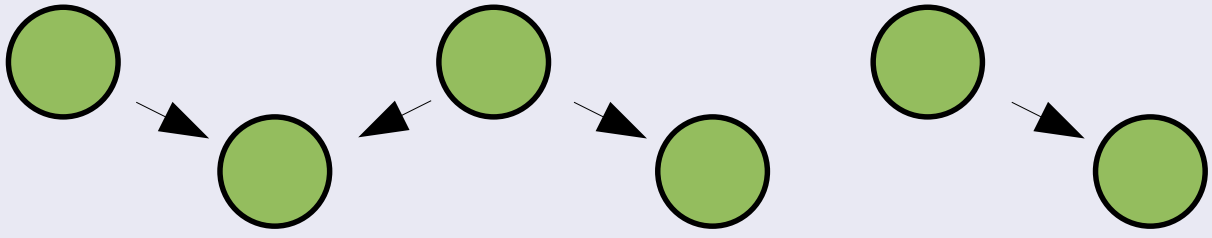
Examples of Linkage Learning EDAs II

Extended Compact Genetic Algorithm (ECGA)



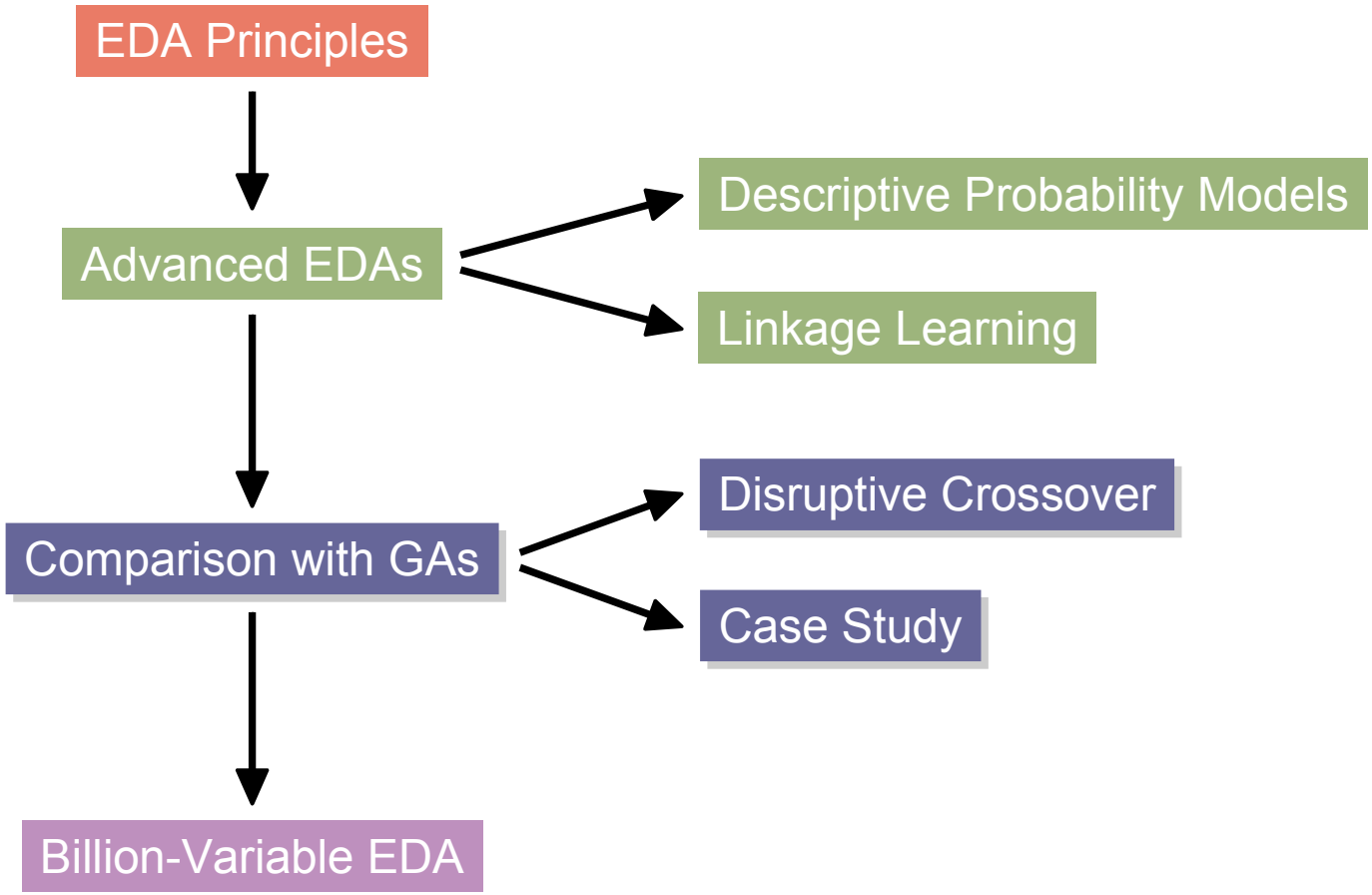
Harik, 1999

Bayesian Optimization Algorithm (BOA)



Pelikan, Goldberg and Cantú-Paz, 2000

Road Map


EDA Principles
Advanced EDAs
Descriptive Probability Models
Linkage Learning
Comparison with GAs
Disruptive Crossover
Case Study
Billion-Variable EDA

Building Blocks

- a *schema* is bit pattern template using the alphabet {0,1,*} where * is a wildcard
- *defining length* is distance between first and last non-wildcard symbols
- *order* is number of non-wildcard symbols

Example

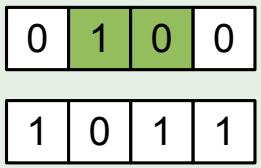
schema: $H = *10*$
representatives: 0100, 0101, 1100, 1101
defining length: $\delta(H) = 1$ order: $o(H) = 2$

- *building blocks* are short, low order, highly fit schemata
- GAs work well when building blocks propogate through the population and are combined to produce fit individuals

Disruptive Crossover

Some crossover operators can disrupt building blocks.

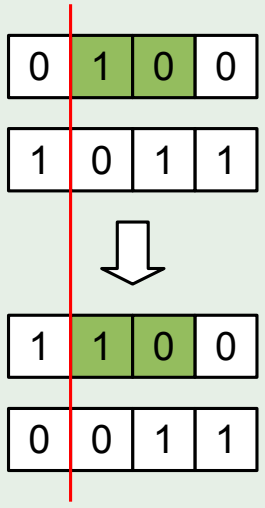
Example - One-Point Crossover



Disruptive Crossover

Some crossover operators can disrupt building blocks.

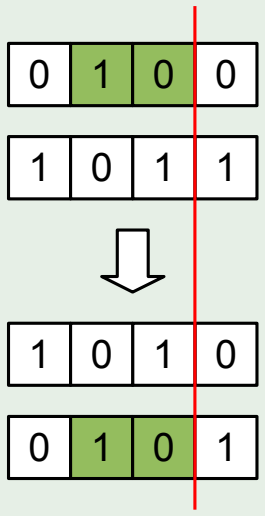
Example - One-Point Crossover



Disruptive Crossover

Some crossover operators can disrupt building blocks.

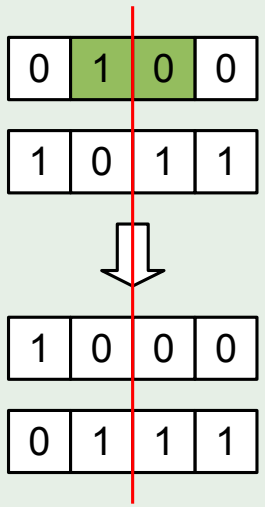
Example - One-Point Crossover



Disruptive Crossover

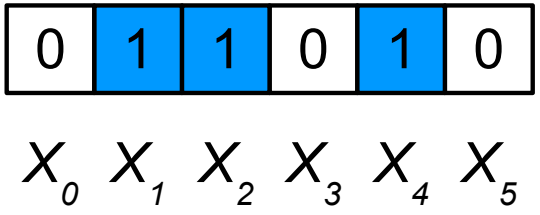
Some crossover operators can disrupt building blocks.

Example - One-Point Crossover



Case Study - Additive Deceptive Function

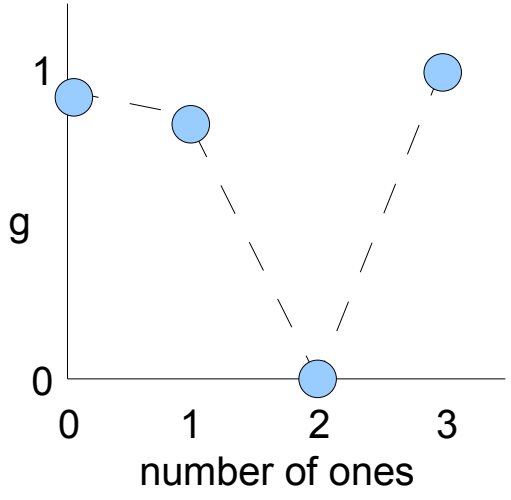
Genome



Fitness

$$f = g(X_0, X_1, X_2) + g(X_3, X_4, X_5)$$

where $g(\cdot)$ is:



global optimum is clearly 111111, but deceptive nature of $g(\cdot)$ tends to move population towards local optimum at 000000

Results Using Standard GA

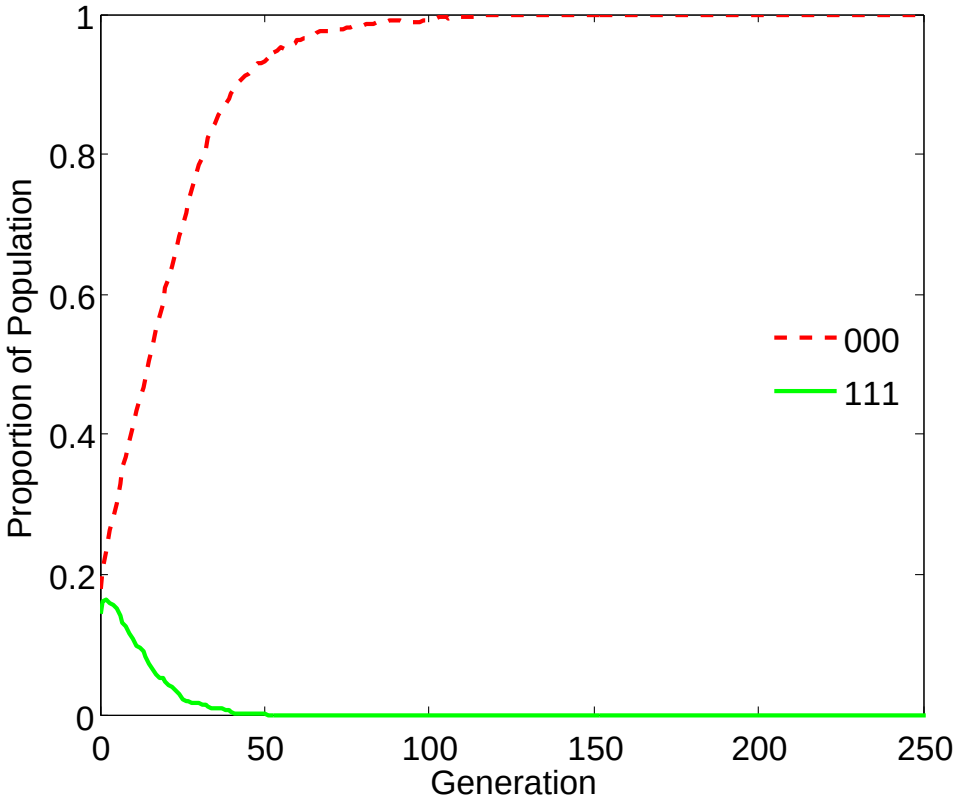
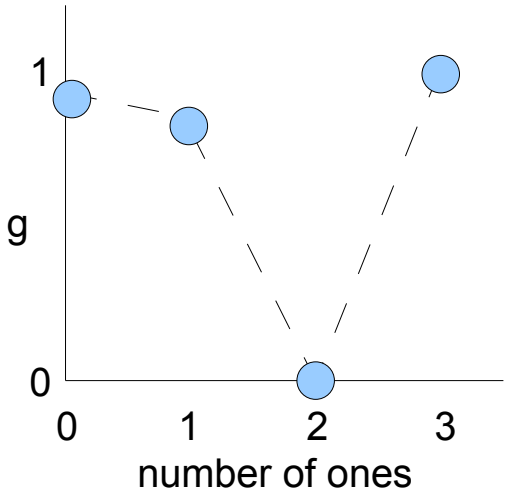
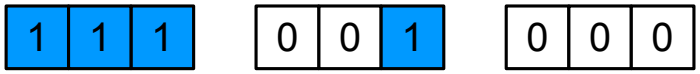


Figure: proportion of population having schemata 111*** and 000*** at each generation; average over 10 runs

- population size 1000
- one-point crossover (with probability 1)
- no mutation
- fitness proportional selection

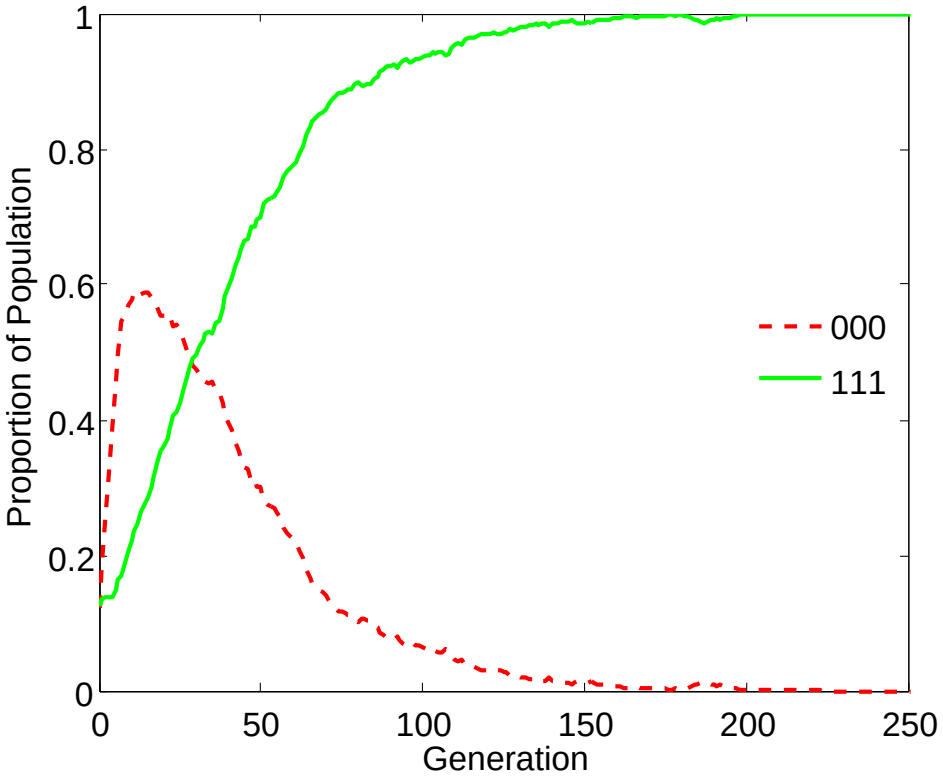
Hypothesis





- schemata with 2 ones are quickly eliminated from population
- crossover between 111 and other schemata is more often destructive than not
- crossover between schemata is unlikely to produce 111
- therefore, schemata with few ones begin to dominate
- since 000 is the fitter of the few ones schemata, algorithm eventually converges to this solution

Results Using EDA



- population size 1000
- fitness proportional selection
- predefined model

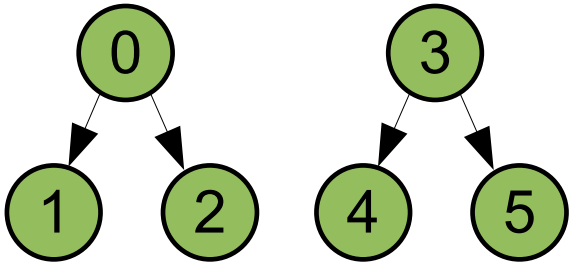
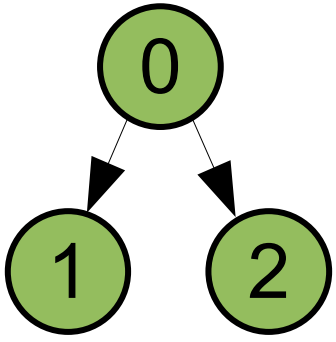


Figure: proportion of population having schemata 111*** and 000*** at each generation; average over 10 runs

Hypothesis I



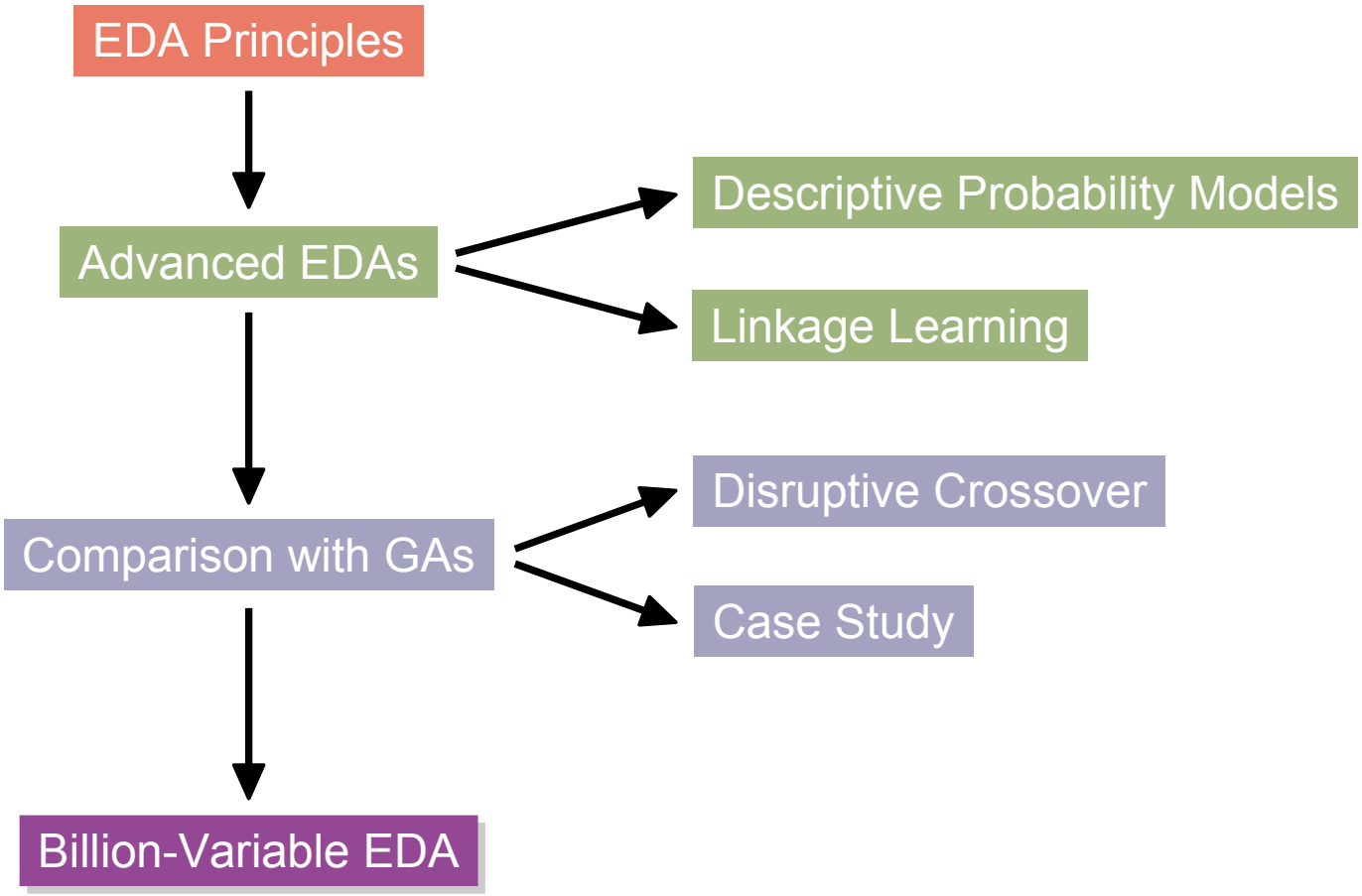
1	0	0	0.8	0	0	0	0.9
1	1	0	0.0	0	1	0	0.8
1	0	1	0.0	0	0	1	0.8
1	1	1	1.0	0	1	1	0.0
			average 0.45				average 0.625

- in initial random population, individuals where $X_0 = 0$ are on average fitter than $X_0 = 1$
- so schemata with $X_0 = 0$ occur more frequently in each new generation

Hypothesis II

- by selection over a number of generations, algorithm then establishes probability distribution for model:
  - given $X_0 = 0$, fitter individuals occur when $X_1 = 0$ and $X_2 = 0$
  - given $X_0 = 1$, fitter individuals occur when $X_1 = 1$ and $X_2 = 1$
- so probability distribution now results in generation of schemata 000 and 111 more often than others
- when this occurs, individuals where $X_0 = 0$ are now on average less fit than $X_0 = 1$
- so 111 schema begins to dominate, and algorithm converges on this solution

Road Map


EDA Principles
Advanced EDAs
Descriptive Probability Models
Linkage Learning
Comparison with GAs
Disruptive Crossover
Case Study
Billion-Variable EDA

Billion-Variable EDA

Towards Billion Bit Optimization via Efficient Genetic Algorithms

Kumara Sastry, David E Goldberg, Xavier Llorà

IlliGAL Report No. 2007007

Illinois Genetic Algorithms Laboratory

University of Illinois at Urbana-Champaign

Best EDA paper award at Genetic and Evolutionary Computation Conference (GECCO) 2007

Problem - Noisy, OneMax

Representation

10^9 variables $x_i \in \{0, 1\}$

Objective

Optimal solution has all $x_i = 1$ ('OneMax')

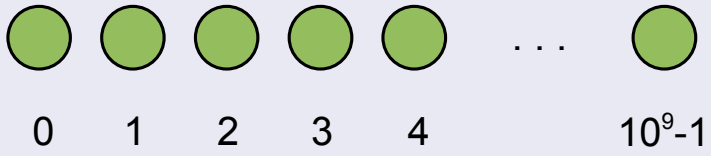
Fitness

$f = \sum x_i + \mathcal{N}(0, \sigma^2)$

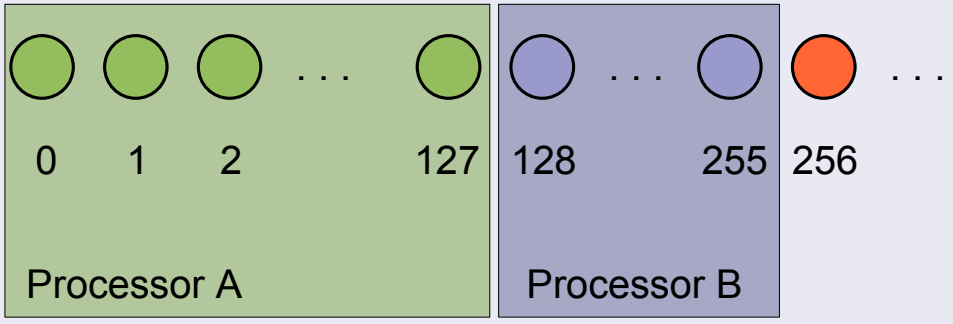
Solution Method

Algorithm

Compact Genetic Algorithm (CGA) - a univariate EDA



Implementation



Results

Extrapolation from Trajectory

For 10^9 variables, algorithm would take too long to converge even on large parallel computing cluster.

Measured time for algorithm to reach point where all probabilities were > 0.501 (from initial probability of 0.5). Extrapolated results from small problems where full convergence was possible.

Novelty

- Real-world problem size
- Very efficient parallel implementation of CGA
- Although simple EDA, superior (more scalable) to other approaches such as hill-climbing on this problem

Summary

- EDAs are a modern form of evolutionary algorithm
- Wide variety of algorithms ranging from simple (e.g. CGA) to advanced, state-of-the-art (e.g. BOA)
- Demonstrate advantages over standard GAs on some problem classes

Selected Resources

Survey of Bit-String EDAs

Martin Pelikan, David Goldberg and Fernando Lobo
A Survey of Optimization by Building and Using Probabilistic Models
IlliGAL Report No. 99018, University of Illinois, 1999

Missouri Estimation of Distribution Algorithms Laboratory

http://medal.cs.umsl.edu/