Is the Common Good?

A New Perspective Developed in Genetic Algorithms

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abstract

Similarities are more important than differences. The importance of these common components is set forth by the commonality hypothesis: schemata common to above-average solutions are above average. This hypothesis is corroborated by the isolation of commonality-based selection. It follows that uncommon components should be below average (relative to their parents).

In genetic algorithms, the traditional advantage of crossover has been attributed to the recombination of (uncommon) parent components. However, the original analysis focused on how the schemata of a single parent were affected by crossover. Using an explicit two-parent perspective, the preservation of common components is emphasized. The commonality hypothesis suggests that these common schemata are the critical building blocks manipulated by crossover. Specifically, common components have a higher expected fitness than uncommon components.

The Commonality-Based Crossover Framework redefines crossover as a two step process: 1) preserve the maximal common schema of two parents, and 2) complete the solution with a construction heuristic. To demonstrate the utility of this design model, domain-independent operators, heuristic operators, and hybrid operators have been developed for benchmark and practical problems with standard and non-standard representations. The new commonality-based operators have performed consistently better than comparable operators which emphasize combination.

In heuristic operators (which use problem specific heuristics during crossover), the effects of commonality-based selection have been isolated in GENIE (a genetic algorithm that eliminates fitness-based selection of parents). Since the effectiveness of construction heuristics can be amplified by using only commonality-based restarts, the preservation of common components has supplied selective pressure at the component (rather than individual) level. This result corroborates the commonality hypothesis--the preserved common schemata are above average.

Transferring the concept of commonality-based selection back to standard crossover operators, beneficial changes should occur more frequently when they are restricted to uncommon schemata. Since multiple parents are required to identify common components, commonality-based selection is an advantage that multi-parent operators (e.g. crossover) can have over single-parent operators (e.g. mutation). These observations present a novel perspective on iterative improvement.

Chapter 1

Introduction

The commonality hypothesis suggests that common components are more important than uncommon components. This new perspective motivates a reexamination of the design influences in genetic algorithms.

1.1 Motivation

Genetic algorithms (GAs) perform iterative improvement--they use existing candidate solutions to find better candidate solutions. During this process, good solution parts should be kept and bad solution parts should be changed. Unfortunately, many iterative improvement techniques focus only on making changes--the changed parts (of a single solution) are assumed to be bad. An explicit attempt to identify good solution parts is often omitted from the search process. To address this omission, crossover in genetic algorithms can use two solutions to actively identify and preserve the good parts. Since traditional (combination-based) models of crossover also omit explicit identification of parent components, the proposed approach to iterative improvement requires a new model of crossover.

1.2 Overview

The commonality hypothesis suggests that schemata common to above-average solutions are above average. To exploit these common schemata, the Commonality-Based Crossover Framework is presented. It defines crossover as a two step process: 1) preserve the maximal common schema of two parents, and 2) complete the solution with a construction heuristic.

The commonality hypothesis and the new design model have been implemented in genetic algorithms. The examined concepts include the Schema Theorem, building blocks, standard and non-standard representations, and the three major categories of crossover operators: domain-independent operators, heuristic operators, and hybrid operators. In theory and in practice, the superior relative fitness of common components is demonstrated.

The Schema Theorem is the original analysis of genetic algorithms. Its interpretation suggests that low-order, highly fit schemata are the critical “building blocks” manipulated by crossover. However, a schema `H` that has `m` (different) examples in a population is equivalent to a schema `H` that is *common* to `m` solutions. Switching from differences to similarities, the analysis used to develop the Schema Theorem can alternatively suggest that common schemata are the critical building blocks manipulated by crossover.

Domain-independent crossover operators (e.g. standard crossover) do not use problem specific knowledge. Although standard crossover operators always preserve common components, early non-standard operators did not. Experiments show that domain-independent operators which use only combination perform better after they are modified to preserve common components.

The definitions of heuristic and hybrid operators have been separated. Heuristic crossover operators incorporate problem specific heuristics into the crossover process. The heuristic is used to select offspring components (from the parents). For heuristic operators, experiments show that transmission and combination can handicap the performance of a problem specific heuristic.

In hybrid GAs, the initial crossover solution (heuristic or domain-independent) is post-processed with a local search technique. A crossover operator-local optimizer pair can be viewed in the aggregate as a hybrid crossover operator. For the same local optimizer, experiments show that a commonality-based heuristic operator can lead to a better overall hybrid operator than other forms of crossover.

The problem domains for the above experiments include vehicle routing, flow shop scheduling, and feature subset selection. In vehicle routing, the developed hybrid operator finds best-known solutions to several library instances. In flow shop scheduling, the performance of the best domain-independent sequencing operator improves when it is modified to preserve (additional) common components. In feature subset selection, a new heuristic operator is more effective than the best standard GAs for binary string representations.

The above experiments also present some general ideas. For example, beneficial search space reductions have been transparently implemented--representation-level constraints are maintained by the preservation of common components. It is also shown that domain-independent design models do not necessarily extend to heuristic operators since transmission and combination can handicap the performance of a problem specific heuristic. Further, heuristic amplification and open-loop optimization are introduced.

The last two effects arise because commonality-based restarts will amplify the effectiveness of a construction heuristic. When the common components of (above-average)

parents are preserved during the first step of the Commonality-Based Crossover Framework, selective pressure is supplied. This new form of selection acts at the component/schema level (rather than the level of individuals), and it is called commonality-based selection.

Using heuristic operators, commonality-based selection has been isolated in GENIE (a genetic algorithm without fitness-based selection at the individual level). When fitness-based "feedback" is removed, this iterative improvement procedure can be viewed as "open-loop" optimization. The existence of commonality-based selection, heuristic amplification, and open-loop optimization corroborates the commonality hypothesis--the schemata common to above-average solutions were above average.

When these above-average (common) components are preserved, beneficial changes become more likely when they are restricted to the remaining below-average (uncommon) components of the parents. Since multiple parents are required to find common components, single-parent operators (e.g. mutation) cannot employ commonality-based selection. Commonality-based selection represents an important advantage that is available to crossover.

1.3 Outline

Chapter 2 provides the necessary background to support the foundation of this thesis. It includes a brief review of evolution and genetics to establish the perceived importance of differences and recombination in these fields. The original development and analysis of genetic algorithms is then introduced.

Chapter 3 is the foundation of this thesis. It focuses on the theoretical effects of the commonality hypothesis (e.g. the Commonality-Based Crossover Framework, commonality-based selection, heuristic amplification, etc). The critical observation is that beneficial changes should occur more frequently when they are restricted to uncommon components. Experimental results to support the new theory are presented in chapters 4-11.

Chapter 4 surveys early domain-independent operators. Since genetic crossover uses no domain-specific information, the development of crossover operators started with this

category. It is shown that the preservation of common schemata (which have superior relative fitness) can improve the performance of domain-independent operators.

Chapter 5 begins the study of heuristic operators--operators which use problem specific heuristics during the development of the (initial) offspring solution. With its directive to use construction heuristics, the Commonality-Based Crossover Framework is the first design model to specifically address this (redefined) category. The developed commonality-based heuristic operators perform better than comparable operators based on combination.

Chapter 6 continues the analysis of heuristic operators. Since these operators are the primary focus of the Commonality-Based Crossover Framework, the largest differences between the new and existing models occur in this category. Through this extended examination, commonality-based selection was first isolated, and heuristic amplification and open-loop optimization were discovered.

Chapter 7 addresses hybrid operators--operators which use local optimizers to post-process an initial offspring solution. It is shown that the quality of the initial start solution (used to seed the local optimizer) can affect the efficiency and effectiveness of the overall operator. Compared to other forms of crossover, the offspring of commonality-based heuristic operators can provide better restart points.

Chapter 8 focuses on vehicle routing problems. Following the Commonality-Based Crossover Framework, Common Clusters are used as the initial partial solution for two problem variations. The effectiveness of the resulting operators supports the general value of common components.

Chapter 9 includes both search space reductions and flow shop scheduling. First, it is observed that commonality-based crossover operators will preserve matched constraints at the representation level. These constraints can be used to (transparently) reduce the search space. When applied to flow shop scheduling problems, Precedence Preservative Crossover with Edges performs better than Uniform Order-Based Crossover--the best previous sequencing operator for order-based objectives.

Chapter 10 examines feature subset selection. Despite the standard representation, an explicit building block analysis is still necessary. Using the commonality hypothesis to differentiate the quality of common components, a heuristic operator is designed that performs better than standard crossover operators.

Chapter 11 analyzes the effects of transmission in heuristic operators. In general, it is suggested that transmission (and combination) are weak/default heuristics. When the domain-independent design principles are super-imposed upon the decision-making process of a problem specific heuristic, the effectiveness of this heuristic can be handicapped.

Chapter 12 summarizes the conclusions. When the preservation of common components supplies selective pressure, the commonality hypothesis must be valid--the schemata common to above-average solution were above average. With the preservation of these (above-average) components, beneficial changes occur more frequently when they are restricted to the (below-average) uncommon components.

Chapter 13 offers a series of possible extensions for the Commonality-Based Crossover Framework and the commonality hypothesis. These extensions focus on future applications where the new concepts may lead to improvements.

Chapter 2

Background

The traditional analysis of crossover (in genetics and genetic algorithms) focuses on recombination--the rearrangement of differences. Single-parent iterative improvement techniques (e.g. simulated annealing and tabu search) focus on changes--the creation of differences. The value of similarities is largely subjugated to the prevailing importance of differences.

2.1 The Natural Metaphors

Genetic algorithms are modeled after processes in evolution and genetics. To understand GAs at an intuitive level, it is useful to understand the basic concepts of these fields. In particular, the perceived importance of differences is founded in evolution, and the primary role of combination is established in genetics.

2.1.1 Evolution

Evolution, or the transmutation of species, is the process by which a population undergoes sequential changes (and improves) over time. It provides useful metaphors for the design of iterative improvement techniques--processes by which candidate solutions change sequentially over time. The two most famous theories of evolution have been developed by Jean Bapiste de Lamarck and Charles Darwin.

Lamarck presented three assumptions to explain the process of transmutation [BA82]:

1. The ability of organisms to become adapted to their environments over the course of their own lifetimes.
2. The ability to pass on those acquired adaptations, such as well-developed muscles, to their offspring.
3. The existence within organisms of a built-in drive toward perfection of adaptations.

The above assumptions were unpopular among naturalists. In addition to being incomplete (e.g. they don't explain speciation), the "drive toward perfection" was seen as mystical and unnecessary. As a more believable mechanism, Darwin proposed natural selection. The basic structure of Darwin's theory of natural selection can be summarized as a series of four observations and two conclusions [BA82]:

> Observation 1: All organisms have a high reproductive capacity. A population of organisms with an unlimited food supply and not subject to predation could quickly fill the entire earth with its own kind. Under optimal conditions, all organisms have an enormous reproductive potential, or capacity for population growth.
>
> Observation 2: The food supply for any population [of] organisms is *not* unlimited. The growth rate of the population tends to outrun the growth rate of the food supply.

Conclusion 1: The result must be continual competition among organisms of the same kind (organisms that have the same food or other resource requirements).

Observation 3: All organisms show heritable variations. No two individuals in a species are exactly alike.

Observation 4: Some variations are more favorable to existence in a given environment than others.

Conclusion 2: Those organisms possessing favorable variations for a given environment will be better able to survive than those that possess unfavorable variations; thus, organisms with favorable variations will be better able to leave more offspring in the next generation. As the number and kind of phenotypes change from one generation to the next, evolution occurs.

Observation 3 and Observation 4 focus on differences. The basis of adaptation is that certain (random) *variations* will be more favorable than others. As will be shown, the development of genetic algorithms extends (implicitly) from the above observations. thus, a focus on differences has also been inherited.

2.1.2 Genetics

In 1866, Gregor Johann Mendel published an analysis of heredity in peas. This study focused on *phenotype* heredity--the inheritance of outward appearances (e.g. plant height). The inheritance of phenotypes results directly from the inheritance of genes. Genes are located on chromosomes--the deoxyribonucleic acid (DNA) molecules that pass from parent to offspring during reproduction.

DNA consists of four nitrogenous bases: adenine (A), guanine (G), cytosine (C), and thymine (T). These components are arranged on a double helix--a sugar-phosphate backbone on the outside and the bases on the inside. The bases come in two pairs: A-T and C-G. For example, every A on one helix must be matched by a T on the other helix. The following is an example of a DNA string that is 12 base pairs in length:

```
helix 1: A C C T G A A G C A A T
         | | | | | | | | | | | |
helix 2: T G G A C T T C G T T A
```

At the molecular level, the base sequence of DNA represents the *genotype* of an organism--its internal appearance. The various protein molecules that can be synthesized from the DNA represent the phenotype of an organism. To transform from genotype to phenotype, the DNA is read as three-letter "words" (of base sequences). Each word defines an amino acid, and properly composed sequences of amino acids form proteins. The DNA "source code" for a single protein is often viewed as a single *gene*.

Chromosomes consist of linear arrays of genes. For (competing) genes of the same *allele* (chromosome location), the specific gene that an offspring receives depends on how the parent chromosomes *cross over* during reproduction. In crossover, chromosomes break, and the broken pieces are exchanged between homologous chromosome pairs. Through this exchange of genes, the offspring receives a *recombination* of parental traits (phenotype expressions).

It is viewed that the "... additional potential for recombining parental traits [during crossover] is a major advantage of sexual reproduction" [BA82]. Conversely, a more specific benefit of recombination is shown by Muller's ratchet [Mul64]. Muller's ratchet is the process by which deleterious (bad) mutations accumulate in a population. In highly evolved organisms, a point mutation (the alteration of a single DNA base pair) will often be bad. For example, altering a single base pair in the gene for (normal) hemoglobin can lead to the production of sickle-cell hemoglobin. Since all populations continuously suffer deleterious mutations, they all suffer decreased fitness as well [Hal37].

In a population that undergoes asexual reproduction, it can be expected that *every* member of the population will eventually have at least one deleterious mutation. Since the probability of back-tracking a mutation is negligibly small, the maximum fitness of the population is irreversibly lowered--the ratchet has clicked. However, with sexual reproduction, two parents, each with one (different) deleterious mutation, have a 25% chance to produce a mutation-free offspring[1]. Thus, the ability to counteract Muller's ratchet clearly demonstrates that recombination is a critical advantage of crossover.

1. The offspring has an independent probability of 50% to receive each of the mutated genes. Therefore, it has a $(50\%)^2$ change to receive neither.

2.2 Genetic Algorithm Basics

A genetic algorithm performs function optimization by simulating the process of Darwinian evolution. Its three basic features are a population of solutions, fitness-based selection, and crossover. In a "classical" genetic algorithm [Hol75], the population is held at constant size. This population is replaced in "generations"--n offspring solutions are created from n parent solutions, and then all of the parent solutions are discarded.

To simulate natural selection, solutions compete for positions in the "mating pool"--the subset of solutions that are allowed to produce offspring. Competition is based on a solution's (phenotype) "fitness"--the value of its objective function. The original method for fitness-based selection is roulette-wheel/proportionate selection--the proportion that a parent's fitness is of the population's total fitness determines its expected proportion in the mating pool. Thus, fitter solutions (organisms with favorable variations) should dominate the mating pool, and they should subsequently propagate more of their genes/ traits onto future generations.

In genetic algorithms, chromosomes (solutions) are represented by binary bit strings--the "standard representation". Modeling DNA strings, these bit strings represent the genotype of a solution. The competing genes for each position (allele) on a string are 1 and 0. These bits (genes) are the atomic unit in GAs (rather than DNA bases). An example of two solutions with length $l = 9$ follows:

$$A_1 = 0\ 1\ 1\ 0\ 0\ 1\ 0\ 1\ 1$$
$$A_2 = \mathbf{1\ 1\ 0\ 1\ 1\ 0\ 1\ 1\ 0}$$

To simulate the recombination of genes during sexual reproduction, genetic algorithms also use crossover. Crossover creates two offspring solutions from two parents by exchanging their bits at homologous positions. For example, if one-point crossover is applied to solution A_1 and solution A_2 with a cut-point after the fourth allele, the resulting offspring are

$$A'_1 = 0\ 1\ 1\ 0\ \mathbf{1\ 0\ 1\ 1\ 0}$$
$$A'_2 = \mathbf{1\ 1\ 0\ 1}\ 0\ 1\ 0\ 1\ 1$$

The transformation from bit strings (genotype) to objective function value (phenotype fitness) has not been specified. By design, the basic mechanisms of a genetic algorithm are independent of any specific problem domain. This allows genetic algorithms to be a general method for function optimization--just like genetic crossover.

Genetic crossover can be applied to any organism that is represented by DNA. Through the new variations caused by (random) recombination, natural selection at the phenotype level causes highly adapted DNA strings (organisms) to evolve. By analogy, it should be possible to optimize any function which can encode its solutions as binary bit strings. Specifically, select parent solutions with high objective values (phenotype fitness), and create new offspring solutions by applying crossover to the bit string representations (genotypes) of the parents. Using fitness-based selection to replace natural selection, better solutions with higher objective values should "evolve" over time.

This analogy is supported by the Schema Theorem. Before presenting the Schema Theorem (see section 2.3), the concept of *schemata* (plural of schema) is introduced. Schemata are similarity templates that describe subsets of solutions which are similar at certain alleles. Using "`*`" as a wildcard that allows a `1` or a `0` to be substituted, each allele may be `{0,1,*}`. Thus, there are $3^9 = 19683$ possible schemata in solutions of length `9`. Examples of schemata in solution A_1 include:

$$H_1 = 0\ *\ 1\ *\ *\ *\ *\ 1\ *$$
$$H_2 = *\ *\ *\ *\ *\ *\ 0\ *\ 1$$
$$H_3 = *\ 1\ 1\ *\ 0\ *\ *\ 1\ *$$

These schemata match solution A_1 at all of their non-wildcard genes. Overall, every solution A_1 is a representative of $2^9 = 512$ different schemata--each allele can have the gene or a wildcard. Thus, a genetic algorithm examines a very large number of schemata with each complete solution. (See section 2.4.)

To introduce some GA-specific terminology, the *defining length* of a schema, $\delta(H)$, represents the number of cut-points that affect the schema (also, the farthest distance between non-wildcard genes), e.g. $\delta(H_2) = 2$. The *order* of a schema, $o(H)$, is the number of specified (non-wildcard) genes in the schema, e.g. $o(H_3) = 4$.

Analyzing the previous example of crossover from the perspective of parent solution A_1, the cut-point affects schema H_1 and H_3. Schema H_3 is *disrupted*, i.e. it appears in neither offspring, but schema H_1 *survives* in offspring solution A'_1 because parent solution A_2 also has a 1 for the eighth allele. The cut-point does not affect schema H_2, so it survives (in offspring solution A'_2).

2.3 The Schema Theorem

Holland's (initial) genetic algorithm operates as follows: (1) start with an initial population of n (random) solutions, (2) select a mating pool of n parents (with replacement) with a bias towards fitter solutions, (3) create a generation of offspring by probabilistically applying (one-point) crossover to each parent, and (4) on this new population, repeat (2) and (3) until a termination condition is met. To follow the effects of these mechanisms on schemata, the Schema Theorem is introduced.

2.3.1 The Original Form

The original Schema Theorem was developed for the standard (binary string) representation, a "generational" replacement scheme, roulette-wheel parent selection, and one-point crossover. For roulette-wheel selection, a solution i with an objective value (fitness) f_i has a probability $f_i/(\Sigma f)$ of being selected, where Σf is the summed fitness of all solutions in the entire population. Visually, spin a roulette wheel with total size Σf made from n sectors f_i in size.

If at time t, there are m examples of a particular schema H in the population $\boldsymbol{B}(t)$, roulette-wheel selection will cause an expected

$$m(H, t+1) = m(H, t) \cdot \frac{f(H)}{\bar{f}} \quad (2.1)$$

examples of schema H to be present in the next generation (at time $t+1$). In equation (2.1), $f(H)$ is the average fitness of the solutions that contain schema H in the population at time t, and $\bar{f} = (\Sigma f)/n$ is the average fitness of all solutions in the entire population $\boldsymbol{B}(t)$. Each of the n (independent) selections for parents (to form the mating pool) repre-

sents an example of schema H with probability $\{m(H,t)\cdot f(H)\}/\{n\cdot \bar{f}\}$, i.e. the total fitness of all solutions with schema H over the total fitness of the entire population.

Substituting $P(H,t) = m(H,t)/n$--the proportion of the population that represent examples of schema H--for $m(H,t)$, equation (2.1) becomes

$$(2.2)\quad P(H,t+1) \;=\; P(H,t)\cdot\frac{f(H)}{\bar{f}}.$$

Although fitness-based selection increases the proportion of above-average schemata in the mating pool, no search is performed by this process. Crossover is a structured, randomized method to exchange information among solutions. The purpose of crossover is to create new solutions with a minimal amount of disruption to the schemata chosen by fitness-based selection.

Disruption was first observed from a one-parent perspective (e.g. [Gol89]). If one parent has a schema H, the expected amount of disruption it will suffer due to crossover is influenced by three factors: the length of the solution, the defining length of the schema, and the probability of crossover. Of the $l-1$ possible cut-points, $\delta(H)$ represents the number that affect the schema H. Thus, an upper bound for the probability of disruption (if crossover occurs) is $\delta(H)/(l-1)$. The probability of survival and the probability of disruption sum to one. Therefore, if the probability of crossover is p_c, then (from the perspective of the first parent) the probability of survival is

$$(2.3)\quad p_s \;\geq\; 1-p_c\cdot\frac{\delta(H)}{l-1}.$$

The inequality arises because the schema H is not disrupted when the second parent (selected randomly) has similar genes at the “disrupted” alleles. These alleles always match when the second parent is also an example of schema H (i.e. schema H is common to both parents). Since disruption can only occur when the first parent mates a second parent that is not an example of schema H, the probability of survival is better estimated by

$$(2.4)\quad p_s \;\geq\; 1-\left[p_c\cdot\frac{\delta(H)}{l-1}\right][1-P(H,t)].$$

Combining equations (2.2) and (2.4), a schema H that fills a proportion $P(H, t)$ of population $\boldsymbol{B}(t)$ is expected to fill a proportion

$$(2.5) \quad P(H, t+1) \geq P(H, t) \cdot \frac{f(H)}{\bar{f}} \left\{ 1 - \left[p_c \cdot \frac{\delta(H)}{l-1} \right] [1 - P(H, t)] \right\}$$

of population $\boldsymbol{B}(t+1)$ in a genetic algorithm with roulette-wheel parent selection and (one-point) crossover. Equation (2.5) is Theorem 6.2.3 in Holland's book [Hol75]. It is the Schema Theorem, or the Fundamental Theorem of Genetic Algorithms.

2.3.2 The Steady-State Form

Many modifications to the original Schema Theorem exist [GL85][Sch87][Rad91][SJ91] [NV92]. However, the primary influences (e.g. combination) on crossover design models still extend from the original version of the Schema Theorem. For the future development of a commonality-based Schema Theorem, only the Schema Theorem for a "steady-state" GA is required. In a steady-state genetic algorithm, solutions are added to and removed from the population one at a time[1].

The steady-state Schema Theorem is shown for GENITOR--a GA in which (both) parents are selected with a linear rank-based bias and the lowest ranking (least fit) population member is removed (not necessarily a parent) [WS90]. With this removal policy, the effect of *elitism* is built in--the best solutions always survive. Further, the selection bias causes the fittest solution to be selected as a parent more often than the median solution (by the bias amount)[2]. The likelihood of selecting other solutions varies linearly with respect to their rank.

The Schema Theorem depends on the actual value of the selection bias. However, to simplify its development, the effects of fitness-based selection are generically represented as a fitness ratio, FR. In roulette-wheel selection, $FR = f(H)/\bar{f}$--the "gain" in

1. Previously, crossover created two offspring from two parents. For a steady-state GA, it can be viewed that one of these solutions is added to the population and the other solution is discarded, or that crossover is modified to create only one offspring.
2. With a bias of 2.00, linear rank-based selection is equivalent to 2-tournament.

proportion that examples of schema H should receive in one generation. The terms are different for linear rank-based selection, but the same notion of gain persists.

The Schema Theorem for a steady-state GA monitors a schema H with $m(H, t)$ examples in the population $\boldsymbol{B}(t)$. This schema can be expected to have

(2.6) $m(H, t+1) = m(H, t) - losses + gains\ from\ schema\ H + other\ gains$

examples after a single solution is created and removed.

In equation (2.6), the *losses* occur when an example of schema H is removed from the population. If the member to be removed is selected randomly, *losses* occur with probability $P(H, t)$. However, since the least fit member of the population is removed, the probability of a loss varies inversely with the fitness ratio. These *losses* have been estimated by

(2.7) $P(H, t)/FR.$

The *gains from schema* H occur if the first parent has schema H, $FR \cdot P(H, t)$, and it is not disrupted. Disruption occurs if the second parent does not have schema H, $1 - FR \cdot P(H, t)$; and the schema H is affected by (one-point) crossover, $\delta(H)/(l-1)$, or it survives in the discarded offspring, $(1/2)[1-\{\delta(H)/(l-1)\}]$. Combining the above terms, the *gains from schema* H have been quantified as

(2.8) $$FR \cdot P(H, t)\left[1-\{1 - FR \cdot P(H, t)\}\left\{\frac{\delta(H)}{l-1} + \frac{1}{2}\left[1-\frac{\delta(H)}{l-1}\right]\right\}\right].$$

The *other gains* occur if two parents, each without schema H, fortuitously create schema H through crossover. This event is relatively difficult to quantify, so it has been dropped as part of the inequality. Substituting equation (2.7) for *losses* and equation (2.8) for *gains from schema* H into equation (2.6), the resulting Schema Theorem for GENITOR (a steady-state genetic algorithm) is

(2.9)

$$m(H, t+1) \geq m(H, t) - \frac{P(H, t)}{FR} + FR \cdot P(H, t)\left[1-\{1 - FR \cdot P(H, t)\}\frac{1}{2}\left\{1 + \frac{\delta(H)}{l-1}\right\}\right].$$

(Note: time *t* represents an entire generation in the original Schema Theorem, but it represents a single new solution here.)

2.4 Effects of the Schema Theorem

The analysis of genetic algorithms starts with the Schema Theorem. Although its original intention was to characterize the effects to schemata, its interpretations (e.g. implicit parallelism, building blocks, and combination) greatly influence the design of crossover operators. These concepts will be reanalyzed in chapter 3 after the development of a new Schema Theorem.

2.4.1 Implicit Parallelism

> "[The Schema Theorem] provides the first evidence of the [implicit] parallelism of genetic plans. *Each* schema represented in the population $\boldsymbol{B}(t)$ increases or decreases according to the above formulation [equation (2.5)] *independently of what is happening to other schemata* in the population." [Hol75]

Implicit parallelism provides a computational leverage that is believed to be unique to genetic algorithms. Specifically, each evaluation provides information (in parallel) on all 2^l schemata that are represented in a solution. With duplicates and disruption, it is estimated that a population of n solutions usefully processes about $O(n^3)$ schemata each generation [Hol75][Gol89]. This $O(n^3)$ of processed schemata is greater than the $O(n)$ cost of evaluating n solutions.

2.4.2 The Building Block Hypothesis

The Schema Theorem refers to all schemata independently. However, low-order schemata are less likely to be disrupted by crossover, so they are more likely to follow the predicted expectations. Thus, an interpretation of the Schema Theorem suggests that (above-average) low-order schemata are the critical "building blocks" manipulated by crossover.

> "Just as a child creates magnificent fortresses through the arrangement of simple blocks of wood, so does a genetic algorithm seek near optimal performance through the juxtaposition of short, low-order, high-performance schemata, or building blocks." [Gol89]

2.4.3 Combination

Implicit parallelism and low-order building blocks support the concept of combination. Therefore, the interpretation of the Schema Theorem also influences crossover design models. If genetic algorithms employ a parallel search for good schemata (building blocks), a necessary function of crossover is combination--the *independently* processed building blocks must be combined into new offspring. For example, if a desirable schema H_1 exists (in one parent) and another desirable schema H_2 exists (in a second parent), then crossover should be able to produce an offspring with both of the desirable schemata.

The concept of combination has received heavy re-emphasis in the literature. Reinforcing views include Syswerda, "... the next step is to combine [good schemata] together in one genome. This is, after all, the overt purpose of crossover." [Sys89], Radcliffe, "Given instances of two compatible [schemata], it should be possible to cross them to produce a child which is an instance of both [schemata]." [Rad91], and Davis, "... the benefits of crossover ... is that crossover acts to combine building blocks of good solutions from diverse chromosomes." [Dav91].

2.5 Crossover Design Models

Genetic crossover performs recombination--offspring are created by combining various genes taken from the parents. A similar role for crossover exists in genetic algorithms--offspring are created by combining various schemata taken from the parents. With standard binary string representations, each allele has only two options--take the gene of the first parent or the second parent. Clearly, a schema common to both parents is taken.

For non-standard representations (e.g. permutation sequences--see section 2.9.2), there are many choices for the definition of alleles, and many choices for how the resulting genes can be combined (see section 4.2). To cover general (standard or non-standard) representations, the concept of combination has been refined by Radcliffe's design principles [Rad91] and by Convergence Controlled Variation [EMS96]. In both of these models, it is suggested that common components should be preserved. Path relinking can also be considered as a crossover design model.

2.5.1 Radcliffe's Design Principles

A total of seven design principles were presented [Rad91]. Three of the principles involve the design of solution representations, one of the principles describes mutation (see section 2.6 for more details), and the last three principles affect the design of crossover operators. Focusing on these three principles, Radcliffe suggested that crossover operators should employ "respect", "proper assortment", and "strict transmission".

The principle of respect dictates the preservation of common components--two parents that have a schema H in common should produce an offspring that also has the schema H. The principle of strict transmission deals with heredity--schemata in the offspring should be inherited from the parents. The principle of proper assortment is equivalent to combination--it should be possible for two non-competing schemata, one from each parent, to both survive in the offspring.

2.5.2 Convergence Controlled Variation

In Convergence Controlled Variation (CCV), the effects of crossover are analyzed from the perspective of the population. The offspring "variations" that recombination can produce are constrained by the (current) diversity of the population. Thus, the composition of genes in the population determines the probability that a given offspring will receive each of the possible genes. These genes can be sampled from the entire population (e.g. BSC [Sys93] and PBIL [Bal95]), multiple parents [Müh91], or two parents. From these alternatives, (two-parent) crossover restricts the offspring to genes that are represented in only two parents[1]. Thus, crossover (with fewer parents) promotes linkage--high-order schemata (of many smaller building blocks) are more likely to be propagated (because common components are preserved) [EMS96]. However, the remaining genes are implicitly combined.

2.5.3 Path Relinking

In path relinking [Ree94], a path is traced between two parents, and the best (fittest) point on this path is returned as the offspring. This process adds local search to the random

1. If the parents have a common gene, the offspring is restricted to taking/preserving it.

sampling of recombination. Otherwise, the final offspring of path relinking is consistent with both of the previous design models.

2.6 Genetic Algorithm Variations

The review of genetic algorithms to this point has focused on crossover, generational replacement, and steady-state replacement. Beyond these basics (which provide sufficient support for the foundation of this thesis), there are many variations (e.g. messy GAs, inversion, multiple populations, etc). However, none of the current GA variations alter the perceived importance of combination in crossover. Nonetheless, mutation is presented to contrast crossover.

Mutation can be applied to an offspring after crossover. For standard representations, mutation flips a bit (from a `1` to a `0`, or a `0` to a `1`). For non-standard representations, mutation should allow any population $\boldsymbol{B}(t)$ to reach all points in the search space [Rad91]. In general, the purpose of mutation (in genetic algorithms) is to maintain population diversity. Mutation is the most frequently used "variation" that appears in GA applications.

2.7 Evolution Strategies

Evolution strategies (ES) are based on asexual reproduction [FOW66][Sch81]. Essentially, offspring are created by making small variations (mutations) to parent solutions. To simulate the higher reproductive capacity of single-celled (asexually reproducing) organisms, the population replacement scheme of a $(\mu+\lambda)$ evolution strategy proceeds as follows: (1) create an initial population of size λ, (2) "truncate" the population by selecting the μ fittest solutions, (3) allow each parent to create λ/μ offspring, and (4) on the offspring population, repeat (2) and (3) until a termination condition is met.

In general, evolution strategies use continuous (real number) values for genes. However, ES can also be applied to discrete valued solution representations. In these cases, it has been argued that evolution strategies can do everything that genetic algorithms can do. Specifically, from a one-parent perspective, crossover is viewed as a "structured" form of mutation.

2.8 Other General Optimization Methods

Many iterative improvement techniques exist. However, only hill climbing, simulated annealing, tabu search, A-Teams, and ant colonies are mentioned in future chapters. The review of general optimization methods is limited to this list.

2.8.1 Hill Climbing

Hill climbing is the basic algorithm for neighborhood search [RK91]. On a given start solution, apply a series of operators that create a "neighborhood" of new solutions. Take the best solution[1] that improves on the start solution, and continue until the current solution is better than all of its neighbors. This final solution will be a local optimum.

Since hill climbing routines have no global perspective, they are also known as "local optimizers"--each solution in a search space is mapped to its nearest locally optimal solution. However, hill climbing results can be unsatisfactory because no attempt is made to find the global optimum. The effectiveness of hill climbing can be improved by restarting the process from several (random) start points.

Hill climbing procedures (and its derivatives) use (one-parent) operators to perform iterative improvement. Solution parts are changed because changes can lead to improvements. However, the desirability of the unchanged parts is not addressed explicitly. This oversight may cause hill climbing procedures to terminate in unsatisfactory local optima.

2.8.2 Simulated Annealing

Simulated annealing (SA) is a local search procedure modeled after the physical process of metal cooling [KGV83]. The fitness of a candidate solution simulates the energy state of a physical substance (that is being annealed). This substance has a natural tendency to transition to lower energy states, but it can also transition to higher energy states with a temperature-dependent probability. At high temperatures, the probability to make (backward) transitions to higher energy states is also high, so transitions are largely random. At lower temperatures, there is a strong bias to make only (forward) transitions

1. In random hill climbing, take the first solution.

to lower energy states. For a slow enough annealing schedule, the physical substance will finish in the ideal (lowest energy) state with a high probability.

To mimic physical annealing, simulated annealing starts with random hill climbing. If a randomly applied operator finds a better solution, that solution is accepted (to become the new base solution). However, if the operator finds a worse solution, that solution is accepted with a "temperature" dependent probability. This artificial temperature also follows a cooling schedule. At high temperatures, worse solutions are accepted with high probability, and SA acts like a random search. At low temperatures, worse solutions are rarely accepted, and SA acts like a standard hill climbing procedure. For a slow enough cooling schedule, simulated annealing will converge with a high probability to the global optimum.

2.8.3 Tabu Search

Tabu search [Glo89] is a "wander around and keep the best" search strategy that lacks the romance of a natural metaphor. The rules of tabu search promote wandering. Starting with the procedure of random hill climbing, the first improving move is taken. If none of the moves cause an improvement, the next best alternative is taken. At the next step, it is quite possible that the only improving move will be back into the local optimum. To avoid becoming trapped in a two-step cycle, inverses of recent moves are made "tabu". For example, if the last move was "east", disallow (make tabu) the "west" move for at least n moves ($n = 7$ is a typical value). By preventing cycles, the "tabu list" (of tabu moves) promotes exploration.

For similar operators, tabu search should escape from local optima faster than simulated annealing. If all the moves back into the most recently visited local optimum are tabu, tabu search can quickly "march out" of the local optimum and towards another region of the search space. Conversely, simulated annealing can probabilistically "bounce around" the old search region for a very long time before escaping. Tabu search is not concerned with the quality of the "final" solution--it is interested in finding the best solution along the way. Specifically, tabu search concentrates its efforts on exploration (not convergence).

2.8.4 A-Teams

A-Teams are a multi-agent (multi-operator) approach based on cooperative strategies found in certain animal societies (e.g. schools of fish and flocks of birds) [TdS92]. Experiments on A-Teams have shown "scale efficiency"--incorporating more (different) operators into the system allows better solutions to be found. However, these experiments also show that the most powerful operator has a dominant role in determining the final solution quality. In fact, the Markov model used to describe A-Teams [dSou93] can also be interpreted as representing an elaborate restart strategy for the most powerful operator. Overall, it appears that the cooperative strategies modeled in A-Teams are better suited to distributed control problems [CT99].

2.8.5 Ant Colonies

Ant colonies are an optimization technique based on the communication processes employed by foraging ants [DMC96]. Assuming that a solution can be represented as a path through a graph, the probability that an edge is traversed by an "ant" is influenced by the amount of "pheromone" deposited on that edge. Typically, only the best solution of a "generation" is allowed to leave pheromone. Then, with the updated pheromone trails, a new generation of ants creates a new generation of solutions. The pheromone communication process allows diversity to be actively controlled.

2.9 Benchmark Problems

There are two benchmark problems that reappear frequently throughout this thesis and throughout the GA literature in general. They are One Max and the Traveling Salesman Problem (TSP). These problems have been used as analysis tools (not for application results). One Max is a GA-specific problem for standard binary string representations. The TSP is perhaps the most studied of all benchmark combinatorial optimization problems. It is particularly important to the study of genetic algorithms because the TSP requires a non-standard representation (i.e. a permutation sequence).

2.9.1 One Max

One Max is a simple binary string problem where the fitness of a solution is equal to the number of 1's that it has. Clearly, the optimal solution is all 1's. The simplicity of this objective function makes it easy to analyze crossover and its effect on schemata--the fitness of which are trivially determined.

2.9.2 The Traveling Salesman Problem

The Traveling Salesman Problem is a sequence-based combinatorial optimization problem. The objective in the TSP is to find the shortest Hamiltonian cycle in a complete graph of n nodes with symmetric edge weights, i.e. $d(c_i, c_j) = d(c_j, c_i)$. Visually, if a salesman has n cities to visit, find the "tour" such that the least distance is traveled--subject to visiting each city once and only once before returning to the start city. Formally, given n nodes c_i with edge weights $d(c_i, c_j)$, find a sequence π of the n nodes such that the following sum is minimized:

$$\min_{\pi} \sum_{k=1}^{n-1} d(c_{\pi(k)}, c_{\pi(k+1)}) + d(c_{\pi(n)}, c_{\pi(0)})$$

The natural representation for a TSP solution is a permutation sequence (π)--a sequence where each symbol (city) appears once and only once. On this representation, standard crossover can create infeasible offspring--some symbols will appear twice, and some symbols will not appear at all. Thus, constraints must be placed on how the symbols are manipulated.

The TSP instances used in this thesis have been taken from TSPLIB[1]. These problems are the five smallest instances used in Reinelt's survey study on practical TSP methods [Rei94]. Each instance represents a real-world (circuit board) application. Reinelt states that real-world TSP instances are more interesting than random or geometric (e.g. att532) instances because they contain more "structure". This structure can cause the local optima to have larger differences in quality. (See Figure 6.4.)

1. http://www.iwr.uni-heidelberg.de/iwr/comopt/soft/TSPLIB95/TSPLIB.html

2.10 Summary

Darwinian evolution is based on the existence of differences and genetic crossover focuses on the recombination of parent differences. Both of these one-parent perspectives were incorporated into the original development of genetic algorithms. One-parent perspectives are also prevalent in several other iterative improvement techniques.

Chapter 3

The Foundation

A single-parent analysis does not match the defining feature of crossover--it is a two-parent operator. Using a two-parent perspective, the role of common components is examined. This analysis leads to the commonality hypothesis, the Commonality-Based Crossover Framework, heuristic amplification, and the isolation of commonality-based selection.

3.1 Overview

From a two-parent perspective, an offspring receives the common schemata of its parents. It is important to propagate these common schemata when they are responsible for the (high) observed fitness of the parent solutions. The *commonality hypothesis* suggests that the above condition is true: schemata common to above-average solutions are above average.

The concern for disruption is reduced by the commonality hypothesis--the critical common schemata can always be preserved. Thus, disruption is not an effect that needs to be emphasized in the development of the Schema Theorem. A new analysis of the Schema Theorem demonstrates that common schemata can also receive increasing trials under the influence of fitness-based selection.

To exploit these common schemata, the Commonality-Based Crossover Framework is presented as a new design model. It appears that this model is the first to directly address the category of heuristic operators--operators which use problem specific heuristics to help select schemata *during* the crossover process. In these operators, the effectiveness of (embedded) construction heuristics can be amplified.

The effect of *heuristic amplification* demonstrates that the preservation of common components can supply selective pressure. This form of selection is called *commonality-based selection*. Acting at the component level, its existence corroborates the commonality hypothesis--the common schemata it selected/preserved were above average (relative to the average fitness of the parents). Commonality-based selection is also shown to be an advantage of standard crossover operators.

If the (set of) common components are above average, then the (set of) uncommon components will be below average. If the likelihood of a beneficial change increases when they are restricted to below-average components, then changes should target uncommon components. Commonality-based selection provides this focus by ensuring that common components are preserved.

3.2 The Commonality Hypothesis

Neighborhood search assumes that good solutions are clustered in (small) “neighborhoods” around other good solutions. By extension, good solutions should also be clustered in the neighborhood of two good solutions. The schema (similarity templates) of a solution define neighborhoods of various size. The schema that most precisely defines the neighborhood of two (parent) solutions is their maximal common schema. This schema should be primarily responsible for the high observed fitness of the two parents.

To generalize the above observation, the commonality hypothesis suggests that schemata common to above-average solutions are above average. With this explicit attempt to identify what makes a good solution good, the commonality hypothesis motivates a review of genetic algorithms. The Schema Theorem and crossover design models are redeveloped from this vantage.

3.3 Reducing the Concern for Disruption

The original Schema Theorem focuses on the disruptive effects of crossover (see section 2.3). However, these effects are observed from the perspective of a single parent. For example, the schema H_3 in parent solution A_1 is affected by the cut-point and eventually disrupted (see section 2.2). Conversely, a two-parent perspective reveals that common schemata are never disrupted by standard crossover operators[1]. (See Figure 3.1.) If these are the critical schemata (as suggested by the commonality hypothesis), then the design influences derived from the original Schema Theorem may be misled by the disruption-based terms.

In addition to the above argument, the following experiment further reduces the concern for disruption. The relationship between disruption and *exploratory power* is examined. In particular, crossover operators with greater exploratory power (higher disruption) often

1. Two-point crossover uses two cut-points, and uniform crossover (effectively) uses a random number of cut-points--each allele in the offspring receives its gene from a randomly chosen parent.

perform better in elitist (steady-state) GAs [Sys89][Esh91][GS94]. There is less risk to exploration when the offspring do not replace their parents.

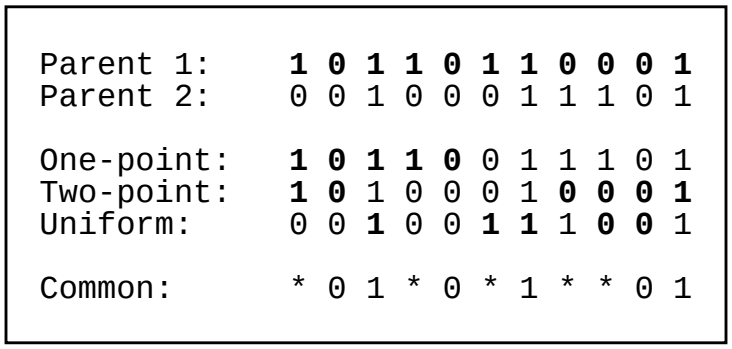


Figure 3.1: Example of standard crossover operators. The offspring solutions are guaranteed to inherit all of the common `1`'s and `0`'s from their parents--regardless of the cut-points.

To demonstrate the greater importance of exploratory power, an objective function highly susceptible to disruption has been designed. In a solution string of 100 bits that is decomposed into 25 blocks of 4 bits each, the fitness increases by 1 if a block is complete--all `1`'s or all `0`'s. If there are *n* adjacent complete blocks of `1`'s (or `0`'s), the fitness increases by n^2. There are two optimal solutions of all `1`'s or all `0`'s (fitness = 625). Crossover causes disruption when it splices a complete block or an adjacent set of complete blocks.

For this objective function, uniform crossover can disrupt more (complete) blocks than both one-point and two-point crossover. In general, the offspring of one-point and two-point crossover were observed to have the same average fitness as their parents. However, the offspring of uniform crossover had an average fitness that was only 70% of their parents[1].

In a generational replacement scheme (2-tournament selection, $p_c = 0.8$), one-point and two-point crossover have similar performance, but uniform crossover performs worse. (See Table 3.1.) Without elitism, disruption can be dangerous. However, when using a strongly elitist steady-state replacement scheme (2-tournament selection, remove

1. In the steady-state GA, this figure is accurate for only the first few generations. After convergence, the offspring also have the same average fitness as their parents.

worst), uniform crossover performs better than two-point crossover which itself performs better than one-point crossover. Elitism allows the exploratory power of uniform crossover to be utilized.

Table 3.1: Performance of one-point, two-point, and uniform on an objective that is highly susceptible to disruption. Results are for the average of 100 runs of 100 generations each when using a population size of 100 solutions.

Operator	Generational GA	Steady-State GA
One-point	34.89	54.99
Two-point	37.45	81.34
Uniform	29.06	98.22

Elitism transforms a highly disruptive crossover operator into a minimally restrictive search operator. Specifically, if the maximal common schema of two parents has n wild-card slots, the exploratory power [ECS89] of one-point crossover includes $2 \cdot n$ possible offspring, two-point crossover can explore $n^2 - n$ possible offspring, and uniform crossover can explore 2^n possible offspring. Since these are supersets, the best possible offspring for two parents under uniform crossover is at least as good as that under two-point crossover which is at least as good as that under one-point crossover.

The above relationship matches the relative performance of the three operators in the elitist GA. With elitist replacement strategies, increased exploratory power is more important than decreased disruption [Sys89][Esh91][GS94]--even in problems with large penalties for disruption. Since these results suggest that disruption is not a (practical) concern, it is removed from the (steady-state) Schema Theorem (see section 2.3.2).

3.4 A Commonality-Based Analysis of the Schema Theorem

Crossover is a two-parent operator. Since crossover is the defining feature of a genetic algorithm, a two-parent perspective should be used to develop the Schema Theorem. From this perspective, the effects to common schemata are easy to observe, and the effects of disruption are easy to ignore. Different design influences extend from the Schema Theorem when these common schemata are highlighted. In particular, combination is no longer supported as the primary mechanism of crossover.

Originally, the effects of fitness-based selection and crossover were examined for a schema H with m examples in a population $\boldsymbol{B}(t)$. A schema H with m examples is equivalent to a schema H that is common to m solutions. Reexamining the effects of fitness-based selection and crossover, the development of the Schema Theorem is reanalyzed by examining a schema H that is common to m solutions in a population $\boldsymbol{B}(t)$.

Starting from equation (2.6) for a steady-state GA, the number of solutions m that have a common schema H is approximated by

$$(3.1)\quad m(H, t+1) \approx m(H, t) - \textit{losses} + \textit{gains from schema } H + \textit{other gains}.$$

If the disruption terms (derived specifically for one-point crossover) are dropped from equation (2.8), the *gains from schema* H become

$$(3.2)\quad FR \cdot P(H, t)[1 - \{1 - FR \cdot P(H, t)\}].$$

Simplifying, it can be seen that the *gains from schema* H occur if and only if both parents have schema H. Thus, these gains are

$$(3.3)\quad [FR \cdot P(H, t)]^2.$$

Since only the disruption terms of equation (2.8) were developed with a one-parent perspective, the gains represented by equation (3.3) implicitly use a two-parent perspective[1]. These gains are also independent of the crossover operator (and the representation)--*any* crossover operator that preserves common components will produce these *gains from schema* H.

Filling in the remaining terms, the *losses* occur if the removed solution contains schema H. Since there are many methods by which this solution can be selected (e.g. worst, tournament, oldest, etc [SV99]), an exact value is less important than an appreciation that the *losses* vary with $P(H, t)$ and inversely with FR. Dropping the *other gains* to form an

1. These gains are equivalently derived from an explicit (crossover independent) two-parent perspective. (See Figure 3.1.)

inequality, the Schema Theorem is reduced to

$$(3.4) \quad m(H, t+1) \geq m(H, t) - f\left(\frac{P(H, t)}{FR}\right) + [FR \cdot P(H, t)]^2 .$$

Although less specific than the original Schema Theorem, it can still be seen that schemata common to a large number of above-average solutions should still receive the desired increasing number of trials.

The intended conclusion of the original Schema Theorem is not actively used (e.g. the exponential allocation of trials is disputed [GB89][Müh97]). However, its influences on crossover design models remain. The desire to combine components from the parents (i.e. building blocks) has not diminished to the extent of the Schema Theorem.

The above analysis is independent of crossover and representation. In the subsequent analysis, the role of combination becomes invisible. However, common components (given that they are preserved) are uniquely capable of *persistence*--a feature that distinguishes "between search like and non-search like processes" [Sha99]. These schemata become the primary focus of the new design model.

3.5 The Commonality-Based Crossover Framework

The commonality hypothesis suggests that common schemata are responsible for the high observed fitness of two parents. A (standard) crossover operator preserves these common schemata and builds an offspring solution from this base (by random recombination). In this functional model, a problem specific heuristic can be used to complete "construction" of the offspring solution. To generalize, the Commonality-Based Crossover Framework defines crossover as a two-step process: 1) preserve the maximal common schema of two parents, and 2) complete the solution with a construction heuristic.

3.6 Other Effects on Genetic Algorithms

The commonality hypothesis suggests that common schemata are the critical building blocks manipulated during crossover. An analysis of crossover probability in generational replacement schemes supports this conclusion. Further, the commonality

hypothesis and the Commonality-Based Crossover Framework do not support the original concept of implicit parallelism.

3.6.1 Crossover Probability in Generational Replacement Schemes

The probability of crossover is less than one ($p_c < 1$) in the original Schema Theorem. Experimentally, GAs with (non-elitist) generational replacement schemes often perform better with $p_c < 1$[1]. The positive effects that $p_c < 1$ can have on the preservation/ propagation of common schemata are reconfirmed by the following representation and crossover independent analysis[2].

Recall that a solution with schema H is selected for the mating pool with a probability $p_m = FR \cdot P(H, t)$. If crossover always occurs ($p_c = 1$), then schema H is only *guaranteed* to survive when both parents have it,

(3.5) $$p_s = p_m^2.$$

However, if $p_c < 1$, then schema H also survives when crossover is not applied to its parent solution,

(3.6) $$p_s = p_m^2 \cdot p_c + p_m \cdot (1 - p_c).$$

Equation (3.6) represents a line between p_m^2 and p_m that is parameterized by p_c. Since $p_m \leq 1$, it follows that $p_m^2 \leq p_m$. Consequently, equation (3.5) will be less than equation (3.6) when $0 \leq p_c < 1$. The common schemata of a population are more likely to survive with $p_c < 1$ than with $p_c = 1$.

Numerically, assume that a schema H is common to the fittest 25% of solutions in a population $\boldsymbol{B}(t)$. If parents are chosen by 2-tournament selection, schema H is expected to

1. For example, the best results for the generational GA presented in section 3.3 occur when $p_c = 0.8$.
2. An equivalent analysis has previously been shown for standard crossover operators [Sch87].

be in $p_m = 7/16$ of the parents. For $p_c = 1$, the probability of survival for schema H is represented by equation (3.5):

$$p_s = (7/16)^2 = 49/256 \cong 19\%. \quad (3.5)$$

Since this is less than the original 25%, schema H is not expected to receive increasing trials. However, if a typical value of $p_c = 0.6$ is used instead [Gol89], then the probability of survival for schema H is represented by equation (3.6):

$$p_s = (49/256)(0.6)+(7/16)(0.4) = 371/1280 \cong 29\%. \quad (3.6)$$

This is greater than the original 25%, and it is much greater than the ~19% when $p_c = 1$. Thus, the probability of crossover has a significant influence on whether or not the common schemata of above-average solutions will receive an increasing number of trials. This result lends support to the claim that common schemata are the critical building blocks manipulated by crossover.

3.6.2 Implicit Parallelism

In the Commonality-Based Crossover Framework, only one schema (the maximal common schema) is actively manipulated during crossover[1]. Thus, the new design model does not promote the (original) concept of implicit parallelism. Instead, crossover is better viewed as a neighborhood search operator--it exploits the common schemata of two parents as a base to explore for better solutions.

3.7 Effects on Construction Heuristics

The Commonality-Based Crossover Framework suggests that common schemata should be preserved during crossover. These common components provide a “confidence measure” to the embedded construction heuristic. Essentially, it is allowed to “back track” its uncommon (incorrect) decisions and refocus its search efforts. With these commonality-based restarts, the effectiveness of construction heuristics can be amplified.

1. Although this schema contains subschemata, they are not used independently during a single application of crossover.

3.7.1 An Intuitive Reason to Preserve Common Schemata

A (greedy) construction heuristic builds a solution one step at a time. At each step, the heuristic can make a correct decision or an incorrect decision. Assuming that a correct decision causes correct (fit) schemata to be selected, the quality of the solution will vary with the number of correct/incorrect decisions[1]. Thus, increasing the number of correct decisions should also improve the quality of the final solution.

Assume that a construction heuristic makes correct and incorrect decisions with a constant ratio. Then, the number of incorrect decisions *made by the construction heuristic* should decrease if it is started from a partial solution--there are fewer steps where the heuristic can make an incorrect decision. If the partial start solution has a higher proportion of correct decisions (fit schemata) than the construction heuristic normally produces, the final solution should have a higher proportion of fit schemata than a solution constructed from scratch. Thus, construction heuristics should be more effective when they are (re)started from partial solutions with high proportions of fit schemata.

The common schemata of two heuristically constructed solutions can form a partial solution with high proportions of fit schemata. For example, consider the Nearest Neighbor construction heuristic for the TSP. This heuristic starts at a random city and travels to the nearest unvisited city at each step. In this process, Nearest Neighbor starts by selecting many short (fit) edges. However, after myopically "painting itself into a corner", a long (unfit) edge must be selected. Compared to the selection of short edges, the selection of long edges depends more on the start city. Therefore, two Nearest Neighbor tours are likely to have the same short edges, but different long edges. (See Figure 3.2.) The partial solution of common edges should have a higher ratio of short to long edges (fit to unfit schemata) than a complete Nearest Neighbor (parent) solution.

1. For deceptive functions, the observed fitness may decrease even though the number of correct decisions is increasing.

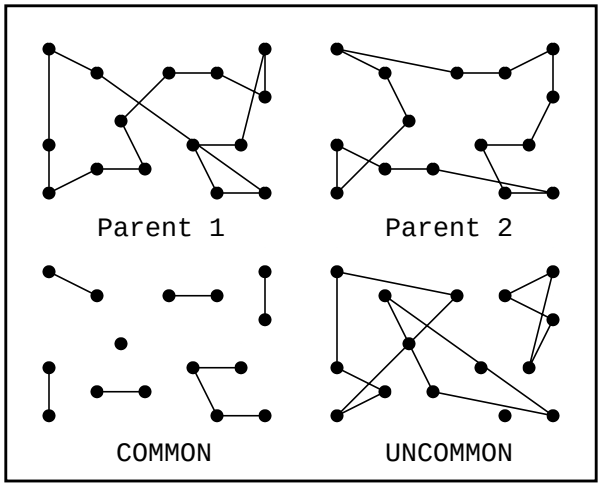


Figure 3.2: Example of two Nearest Neighbor (parent) solutions constructed from different start cities. Their common edges tend to be short (nearest neighbor) edges, and their uncommon edges tend to be long/crossing edges.

3.7.2 Heuristic Amplification

To analyze the potential increase in effectiveness available from a commonality-based restart, assume that each (binary) decision of a construction heuristic is *independent* (unlike Nearest Neighbor in which the selection of long edges *depends* on previous decisions). Further, assume that it makes correct decisions (i.e. selects schemata that are part of the optimal solution) with probability p and incorrect decisions with probability $1 - p$. If this heuristic is used to generate the initial population, each (parent) solution is expected to have a proportion p of correct decisions, and a proportion $1 - p$ of incorrect decisions. For random parent selection, Table 3.2 shows the expected distribution of correct/incorrect and common/uncommon decisions for parent pairs taken from the initial population.

Table 3.2: Expected distribution of decisions for random parent pairs in the initial population.

	p correct	1-p incorrect
p correct	p^2 common correct	p(1-p) uncommon
1-p incorrect	p(1-p) uncommon	$(1-p)^2$ common incorrect

Among the common decisions, the ratio of correct to incorrect decisions is $p^2/(1-p)^2$. If the construction heuristic makes more correct decisions than incorrect decisions (i.e. $p > 0.5$), then $p/(1-p) > 1.0$ and

$$\frac{p^2}{(1-p)^2} > \frac{p}{1-p}.$$

The common-schema partial solutions have a higher ratio of correct to incorrect decisions than (parent) solutions of the initial population[1]. When these components are preserved, a (non-random and productive) form of selection occurs that is *not based on fitness*. Relative to the components generated by the construction heuristic, the subset of components identified by commonality are expected to be above average.

Numerically, the proportion of correct decisions in the initial population is $c_0 = p$, and the proportion of incorrect decisions is $\bar{c}_0 = 1-p$. To extend the analysis, assume that the above construction heuristic is embedded into a heuristic operator by following the Commonality-Based Crossover Framework. Specifically, preserve the common components of two parents, and complete the offspring solution from this partial solution with the previous construction heuristic.

Using a GA with random parent selection and generational replacement for the above operator, the correct decisions in generation i are the common correct decisions from generation $i-1$ and the correct decisions made by the construction heuristic during generation i. To simplify the analysis, assume that the construction heuristic generates a *constant* proportion p of correct decisions (i.e. the construction heuristic is *ideal*). For this model, the expected proportion of correct decisions c_i in generation i is

$$c_i = c_{i-1} \cdot c_{i-1} + p[2 \cdot c_{i-1} \cdot \bar{c}_{i-1}]. \quad (3.7)$$

1. For non-binary decisions, the number of incorrect decisions is usually be greater than the number of correct decisions. Thus, $(1-p)^2$ should be a high estimate of the proportion of common incorrect decisions, and the ratio of correct to incorrect decisions among common components will often be even higher.

Simplifying,

$$c_i = c_{i-1} \cdot (c_{i-1} + 2p \cdot \bar{c}_{i-1})$$

Representing $p \in [0,1]$ as $0.5(1 + x)$, $x \in [-1,1]$;

$$\frac{c_i}{c_{i-1}} = c_{i-1} + 2p \cdot \bar{c}_{i-1}$$

$$\frac{c_i}{c_{i-1}} = c_{i-1} + (1 + x) \cdot (1 - c_{i-1})$$

$$\frac{c_i}{c_{i-1}} = c_{i-1} + 1 - c_{i-1} + x - xc_{i-1}$$

$$\frac{c_i}{c_{i-1}} = 1 + x(1 - c_{i-1})$$

If $p > 0.5$, then $x > 0$ and $c_i > c_{i-1}$. The proportion of correct decisions in the population increases with each generation when $p > 0.5$. For a commonality-based restart to be productive, the ratio of correct to incorrect decisions generated by the construction heuristic needs to be greater than 1 (but not necessarily constant).

At convergence, $c_* = c_i = c_{i-1}$. Substituting c_* into equation (3.7) leads to

(3.8) $$c_* = c_*^2 + p[2 \cdot c_* \cdot (1 - c_*)]$$

$$c_* = c_*^2 + 2pc_* - 2pc_*^2$$

$$c_*(1 - 2p) = c_*^2(1 - 2p)$$

The equality in equation (3.8) requires $c_* = 0$, $c_* = 1$, or $p = 0.5$.

For $p > 0.5$, c_i converges to 1 (all solutions in the population are optimal). However, c_i converges to 0 for $p < 0.5$. (See Figure 3.3.) Therefore, the effectiveness (or ineffectiveness) of construction heuristics is amplified by commonality-based restarts. This effect is called *heuristic amplification*.

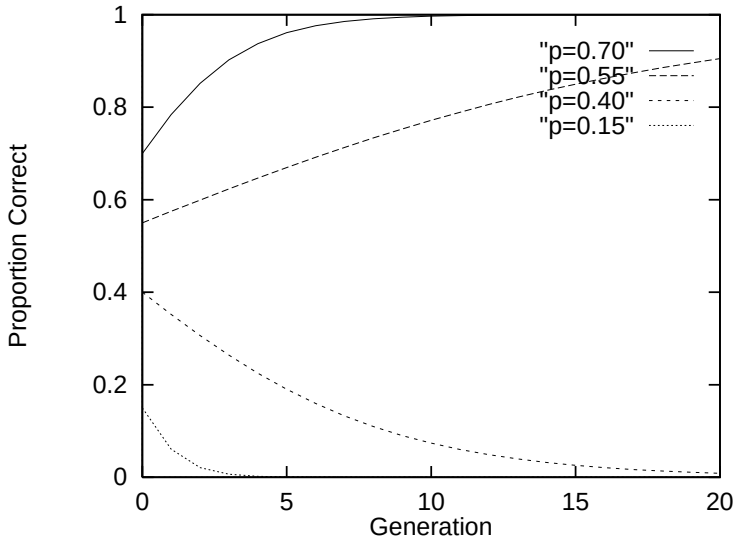


Figure 3.3: Expected proportion of correct decisions in generation `i` for commonality-based crossover operators encapsulating ideal construction heuristics with different `p`.

3.8 Commonality-Based Selection

Populations and/or fitness-based selection are used by many iterative improvement techniques. However, only genetic algorithms use crossover. "[Crossover] is regarded as the distinguishing feature of [genetic] algorithms ... and as a critical accelerator of the search process" [Dav91]. Traditionally, the advantage of (genetic) crossover has been attributed to the mechanism of combination. Thus, crossover operators have been based on recombination.

The first step of the Commonality-Based Crossover Framework dictates that common schemata should be preserved. Essentially, they are *selected* to survive in the offspring. In heuristic operators, the preservation of common components supplies a selective pressure that leads to heuristic amplification. To demonstrate that commonality-based selection is an advantage of standard crossover, its effects are analyzed for One Max[1].

A One Max solution with above-average fitness will have more `1`'s than `0`'s. If a random mutation is applied to this solution, it will most likely turn a `1` into a `0` (rather than the

1. In "decision space", all binary string problems reduce to One Max--`1`'s represent correct bits, and `0`'s represent incorrect bits.

reverse). For randomly selected bits, beneficial mutations are less likely than deleterious mutations. However, these odds improve if common components are preserved.

```
Parent 1:       1 0 1 1 0 1 0 1 1 1
Parent 2:       1 1 0 1 0 1 1 1 0 1

Common:         1     1 0 1   1   1

Uncommon 1:       0 1       0   1
Uncommon 2:       1 0       1   0
```

Figure 3.4: Example of commonality-based selection. There is a higher ratio of `1`'s to `0`'s among the common alleles--the schemata identified by commonality-based selection are indeed above average. Subsequently, a beneficial mutation is more likely if mutations are restricted to uncommon schemata only.

Assume that two One Max (parent) solutions each have seven `1`'s and three `0`'s (all *randomly* distributed). Each allele has a 0.7*0.7 = 49% chance that both parents have `1`'s, a 9% chance that both parents have `0`'s, and a 42% chance that the parents will be uncommon. (See Table 3.2.) Overall, there should be five alleles with common `1`'s, one allele with a common `0`, and four uncommon alleles--two `1`'s and two `0`'s. (See Figure 3.4.)

For a random mutation (to either parent), there is a 70% chance of going backwards (turning a `1` into a `0`), and only a 30% chance of going forwards. However, if mutation is restricted to uncommon bits only, then the chance of going forwards is 50%. Specifically, a beneficial mutation is more likely if mutation is restricted to the uncommon bits.

To identify common schemata, multi-parent operators (e.g. crossover) must be employed. Therefore, commonality-based selection is an advantage that crossover can have over one-parent operators. To benefit from this advantage, crossover operators must be designed to preserve common components.

3.9 The Critical Observation

If the common components are above average (relative to the complete set of components which represent a parent solution), then the uncommon components will be below

average. Since the likelihood of a beneficial change can increase when they are restricted to below-average components, changes should target uncommon components. Commonality-based selection provides this focus by ensuring that common components are preserved.

3.10 Summary

The commonality hypothesis presents a two-parent perspective for the analysis of crossover. It suggests that common components are the critical building blocks manipulated by crossover. Following this suggestion, the Commonality-Based Crossover Framework is introduced. Its directive to preserve common components provides an additional form of selection. Compared to one-parent operators, crossover can have the advantage of commonality-based selection.

Chapter 4

Domain-Independent Operators

Standard crossover is a domain-independent operator. Although it preserves common schemata, several early non-standard operators did not. The preservation of common schemata (which have superior relative fitness) can improve the performance of these operators.

4.1 Overview

The standard crossover operators are domain independent. As the actions of biological crossover on DNA are independent of the organism, the actions of standard crossover operators are independent of the objective function. This domain independence allows genetic algorithms to be a general method for function optimization.

From the original Schema Theorem, fitness-based selection causes the proportion of fit schemata to increase over time. Since this effect does not require the explicit identification of fit schemata, an analysis of the manipulated schemata has often been omitted from operator design. As *domain-independent* operators, they should be effective regardless of what the schemata represent!

Crossover operators in genetic algorithms rarely have the same domain independence as genetic crossover. In general, the relative performance of "domain-independent" operators *depends* on the domain. For example, sequencing operators designed for flow shop scheduling are ineffective on the Traveling Salesman Problem, and vice versa. Therefore, these operators are more accurately described as "blind" operators--the fitness of the manipulated schemata cannot be "seen".

The commonality hypothesis and the new design model do not affect blind operators for standard representations--they all preserve common schemata. However, several blind operators that have been designed for the Traveling Salesman Problem (and its permutation sequence representation) do not preserve common schemata. Although operators that preserve common components have since been developed (e.g. Generalised N-point Crossover [RS92]), it is still insightful to review the mechanisms of these earlier operators.

The early sequence-based operators attempt to combine building blocks taken from each parent. However, due to the nature of the representation, it is possible that the common components of two parents are taken from neither. Subsequently, these operators cannot benefit from commonality-based selection.

To examine the effects of commonality-based selection in blind operators, an early sequence-based operator (Order Crossover [Dav85a][OSH87]) is modified to preserve common components. The new "commonality-based" operator (Maximal Sub-Tour

Order Crossover) performs better. Compared to randomly selected schemata (edges), common schemata have superior relative fitness.

4.2 A Review of Sequence-Based Crossover Operators

The standard crossover operators cannot be directly applied to permutation sequences. Since each symbol must appear once and only once, the random swapping of parts between two parents can lead to infeasible offspring. (See Figure 4.1.) To ensure that feasible offspring are produced, crossover must include a constraint handling mechanism.

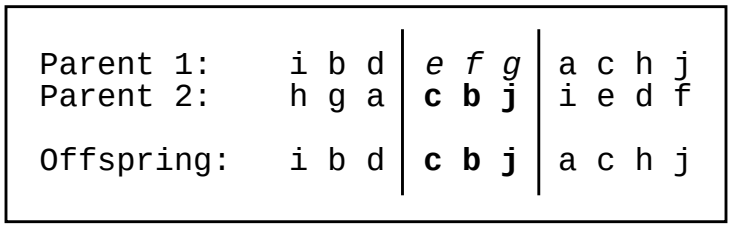


Figure 4.1: Example of standard (two-point) crossover on a permutation sequence. The offspring is infeasible because the cities `c`, `b`, and `j` appear twice, and the cities `e`, `f`, and `g` are omitted entirely.

The building blocks that are manipulated by crossover are (implicitly) defined by the design of the constraint handling mechanism. Specifically, a permutation sequence can represent position-based schemata, edge-based schemata, or order-based schemata. Blind operators for the TSP have been designed with each of these interpretations for schemata. However, the objective for the TSP is primarily edge-based (and secondarily order-based). Since position-based schemata do not match the “building blocks” of the objective, they represent an inappropriate choice for the design of TSP operators.

4.2.1 Position-Based Schemata

Position-based schemata interpret a permutation sequence as a series of independent slots. If the cost (fitness) to assign a city (gene) to a given position (allele) is independent of the cities assigned to the neighboring positions[1], then position-based schemata would be appropriate. However, the (edge-based) objective of the TSP does not satisfy this

1. For example, bin packing problems and assignment problems can have this independence.

independence condition. Operators that manipulate position-based schemata tend to perform poorly on the TSP.

Partially Mapped Crossover (PMX) [GL85] has the form of two-point crossover. The offspring takes the cities from Parent 2 between the cut-points, and it takes the cities in the first and last sections from Parent 1. However, if a city in these outer sections has already been taken from Parent 2, its "mapped" city is taken instead. The mappings are defined between the cut-points--the city of Parent 2 is mapped to the corresponding city of Parent 1. (See Figure 4.2.)

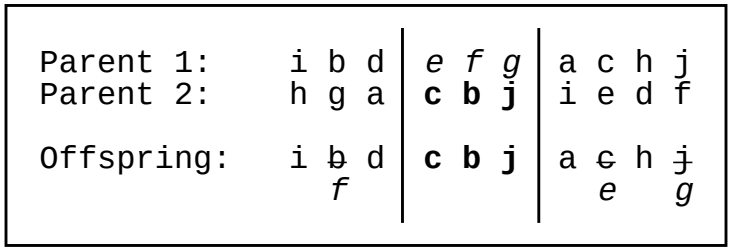


Figure 4.2: Example of PMX. The mappings are c-e, b-f, and j-g.

From the perspective of position-based schemata, the two parents suggest that items b and f are both good fits for the fifth "bin". Therefore, items b and f should have compatible features (e.g. size). Swapping the location of these items creates a (neighboring) solution that might fit the items more successfully into the available bins. For position-based schemata, a PMX offspring receives common mappings (of items into bins) from the parents. Unfortunately, the objective of the TSP (unlike the objective for bin packing) has little to do with fitting items into bins, and the more appropriate adjacency relationships have been ignored by PMX.

For the TSP, PMX was presented as a "sub-tour" operator. The sub-tour of cities between the cut-points in Parent 2 is transplanted into Parent 1. However, the sub-tour taken from Parent 2 might not be fit or (more importantly) fitter than the sub-tour in Parent 1. Further, other sub-tours in the first and last sections of Parent 1 can be disrupted when the middle sub-tour is "scattered". As a sub-tour operator, PMX does not consider common sub-tours, and it transmits other sub-tours so poorly that it is difficult for them to be combined.

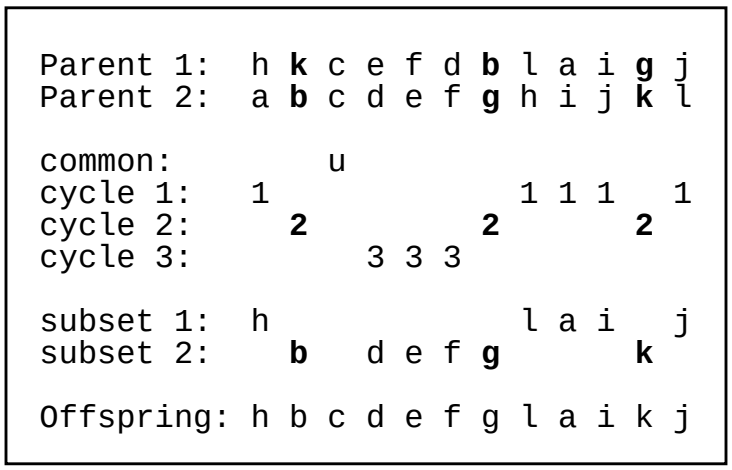


Figure 4.3: Example of CX. Subset 1 has the alleles of cycle 1, and subset 2 has the alleles of cycle 2 and cycle 3. The genes from subset 1 are taken from Parent 1, and the genes of subset 2 are taken from Parent 2.

Cycle Crossover (CX) [OSH87] uses “cycles” to ensure that feasible offspring solutions are produced. A cycle is a set of positions (alleles) that have the same cities (genes) in both parents. Unary cycles (common cities) are transferred directly, and the remaining are split into two subsets. One parent provides the genes for each subset. (See Figure 4.3.) Unfortunately, the building blocks manipulated by Cycle Crossover do not match the edge-based objective of the TSP.

4.2.2 Edge-Based Schemata

Edge-based schemata interpret a permutation sequence as a series of adjacency relationships. If the permutation sequence represents the order in which cities should be visited, the salesman will travel the distance between each pair of adjacent cities. Thus, the edges (between the adjacent cities) make logical building blocks for the TSP. Specifically, fit solutions should be composed of fit (short/low-weight) edges.

Edge Recombination (ER) [WSF89] uses an intermediate representation to process the parent sequences into an offspring solution. This “edge map” lists the cities that are adjacent to a city (preceding or succeeding) in either of the parents. Each city is adjacent to 2, 3, or 4 other cities. To build the offspring, choose the city (in the current edge map) that has the fewest remaining options in its edge map. (See Figure 4.4.)

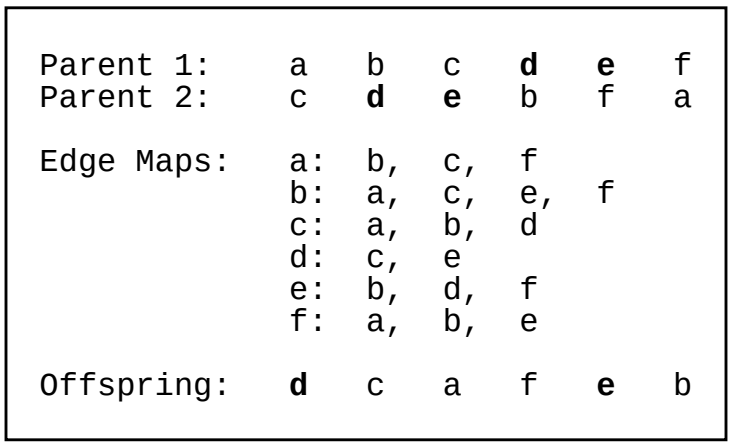


Figure 4.4: Example of ER. Start with city d because its edge map has only two remaining choices. From these choices, (randomly) pick city c to visit next. The updated edge map for city c is c: a, b, ~~d~~. Since city a has only two remaining choices, versus three choices for city b, city a is chosen. In the final offspring, the common edge d-e is disrupted, and the new edge b-d is added (mutation).

Edge Recombination manipulates edge-based schemata (i.e. edges)--parent edges are transmitted to the offspring where they are combined. From this original version, ER has been modified to preserve more common edges (e.g. [SMM91]). With each modification, more common edges are preserved and the performance of the operator improves. Since the latest version of ER preserves all common edges [MW92], a commonality-based form of ER has essentially been developed.

4.2.3 Order-Based Schemata

Order-based schemata interpret a permutation sequence as a series of relative position relationships (e.g. before and after). Although the objective for the TSP is edge-based, there is an implicit order-based aspect to this objective when the edge weights represent physical distances. For example, if there are two clusters of cities, one on the east coast and one on the west coast, the cities on the east coast should be visited *before* the cities on the west cost, or vice-versa. Thus, good order relationships (schemata) can be useful for geometric TSPs.

Order Crossover (OX) [Dav85a][OSH87] has the form of two-point crossover. The offspring starts by taking the cities of Parent 2 between the cut-points. Then, starting from the second cut-point, the offspring takes the cities of Parent 1 (“wrapping around” from the last segment to the first segment). When a city that has been taken from Parent

2 is encountered, it is skipped--the remaining cities are appended in the *order* they have in Parent 1. (See Figure 4.5.)

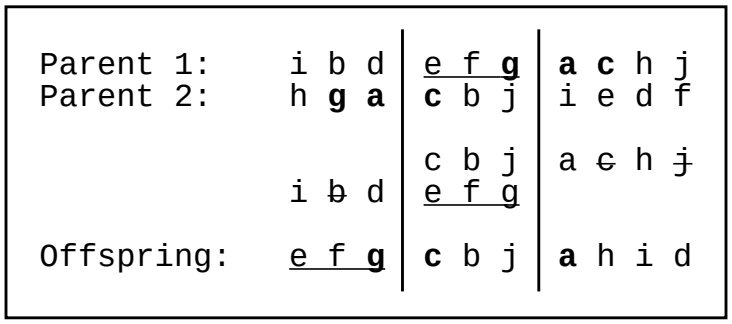


Figure 4.5: Example of OX. Compared to PMX, OX can be less disruptive to sub-tours. For example, the sub-tour `e-f-g` in Parent 1 is now transmitted to the offspring. However, the common sub-tour `g-a-c` is (still) disrupted.

Order crossover assumes that good solutions consist of good sub-tours and/or good order. Thus, OX combines a sub-tour taken from Parent 2 with order taken from Parent 1. Beyond the asymmetry of these actions, common sub-tours and common order are not considered during the recombination process.

The above operators all use a "natural" (symbolic) representation for sequences. However, sequences can also be represented by binary matrices. For example, a $n \times n$ Boolean matrix represents order-based schemata. Element $(i, j) = 1$ if city j follows city i in the sequence[1], otherwise element $(i, j) = 0$. A feasible solution requires three constraints to be satisfied. First, the order must be complete: there are $n(n-1)/2$ ones. Second, transitive order is maintained: if element $(i, j) = 1$ and element $(j, k) = 1$, then element $(i, k) = 1$. Third, there are no cycles: element $(i, i) = 0$ for all i.

If two feasible matrices are intersected (i.e. only common order relationships are preserved), a matrix satisfying the last two constraints is created. This under-constrained "intersection" matrix can be completed by adding random 1's (with an analysis of row/column sums to ensure feasibility). The result is the Matrix Intersection operator (MI) [FM91]. (See Figure 4.6.) Due to the matrix representation, MI has an $O(n^2)$ time

1. A random city is usually fixed for the first position of all solutions.

complexity--much slower than the O(n) time complexity of the previous operators. In addition to their intuitive appeal, natural representations often have time and space advantages over binary representations.

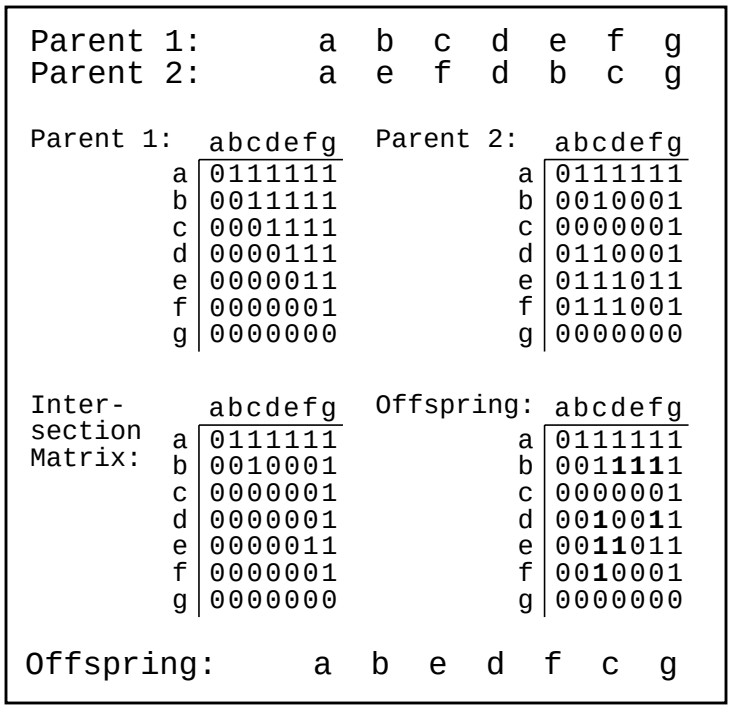


Figure 4.6: Example of Matrix Intersection operator.

The Matrix Intersection operator preserves all common order relationships. However, unlike Order Crossover, MI does not wrap around. Since MI implicitly interprets the sequence as a “path” (where the start city is not revisited) rather than a “cycle”, it performs better on Hamiltonian path problems like flow shop scheduling (see chapter 9). Unfortunately, it performs rather poorly on the TSP.

4.3 Preserving Common Components in Sequence-Based Operators

If an operator does not preserve common components, it cannot benefit from commonality-based selection. To isolate its effects in blind operators, an existing sequence-based operator has been (minimally) modified to preserve common components. Commonality-based selection is responsible for the improved performance.

4.3.1 Maximal Sub-Tour Order Crossover

Order Crossover (OX) assumes that good sub-tours can be extracted from the parents and used to build better offspring. By the commonality hypothesis, an above-average sub-tour that can be taken is the Maximal Sub-Tour (MST)--the longest (undirected) sub-tour that is common to both parents. Thus, OX is modified to preserve the MST.

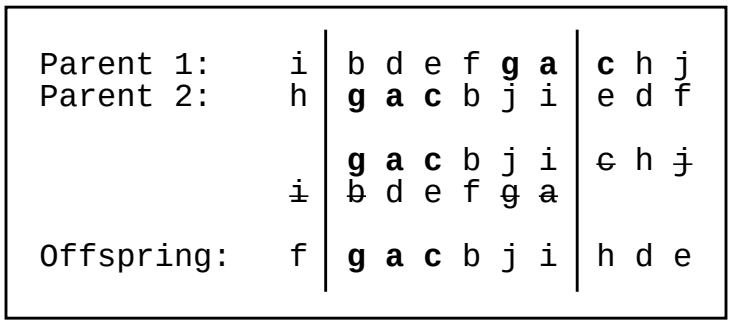


Figure 4.7: Example of MST-OX. The Maximal Sub-Tour g-a-c is now preserved.

After scanning both parents to identify the Maximal Sub-Tour, the first cut-point occurs to the immediate left of the MST in Parent 2. The second cut-point is then made a random distance to the right of the MST[1]. (See Figure 4.7.) Maximal Sub-Tour Order Crossover (MST-OX) then continues with the regular "appending" procedure of Order Crossover. Except for the explicit preservation of the MST, the new operator is identical to OX.

4.3.2 Results: MST-OX vs. OX

The commonality hypothesis suggests that common sub-tours should be shorter than uncommon sub-tours. To measure the relative fitness of a sub-tour, the average edge length of the sub-tour can be divided by the average edge length of the entire (parent) sequence[2]. This ratio for relative fitness is expected to be 1.00 for random schemata, and a ratio of less than 1.00 is expected for above-average schemata.

---

1. For the second cut-point, wrap around is allowed. Virtually, the start position of the MST is "rotated" to become the first position of the sequence.
2. Since the TSP is a minimization problem, this ratio is actually relative cost: (sub-tour length/sub-tour edges) / (total length/n). Relative cost and relative fitness have an inverse relationship.

In OX, the expected ratio of 1.00 is observed for the random sub-tours that are taken from Parent 2. (See “OX_ratio” in Figure 4.8.) Conversely, the “MST_ratio” tends to be less than 1.00--this represents the expected higher relative fitness/lower relative cost for the common components of above-average parents. Although the overall sub-tour taken from Parent 2 includes additional (random) components, the “MST-OX_ratio” still tends to be less than 1.00. Therefore, the transplanted sub-tour in MST-OX is above average (relative to the average fitness of sub-tours in Parent 2).

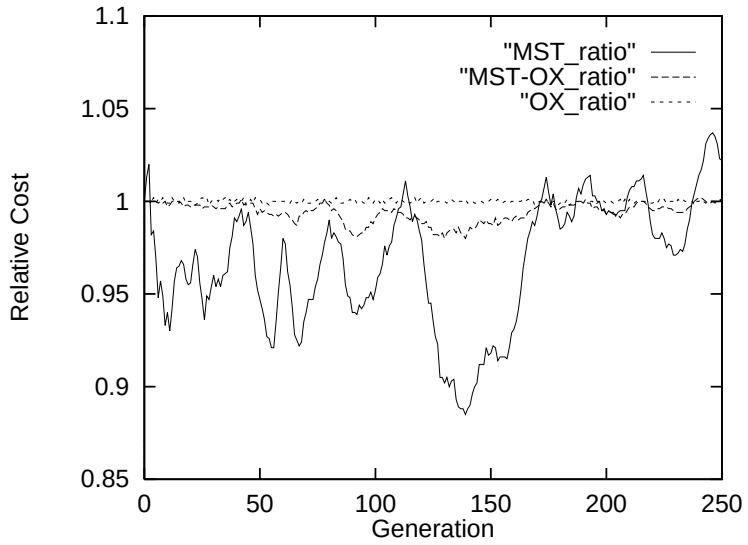


Figure 4.8: Relative fitness. The graph shows the average relative fitness of various sub-tours for each generation during a single run on the lin318 instance. A lower relative cost equates to a higher relative fitness.

From the perspective of sub-tours, the (order-based) appending procedure of Order Crossover causes (random) “mutations”. These mutations are restricted to the less-fit (uncommon) sub-tours in MST-OX, so beneficial changes should occur more frequently (see section 3.9). Specifically, the offspring of MST-OX should be fitter than the offspring of OX. (See Figure 4.9.) However, the average ratio of offspring length to parent length is always greater than 1.00 for both operators--the average offspring is less fit than its parents.

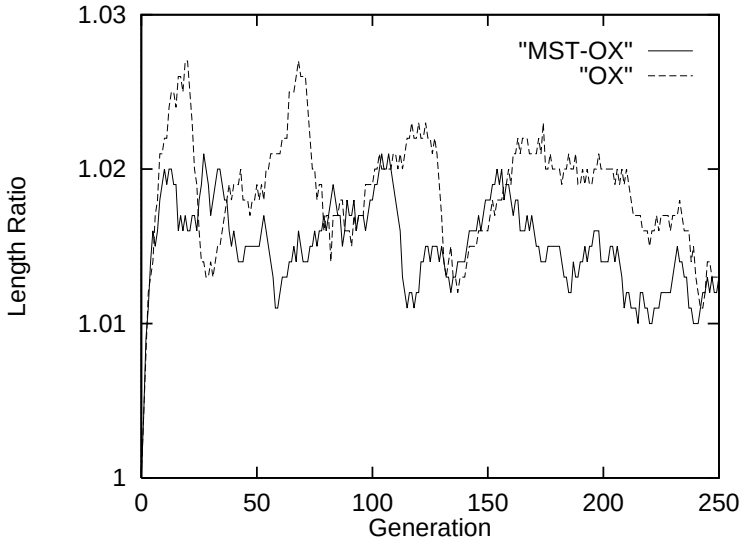


Figure 4.9: Ratio of offspring length to parent length. The graph shows the average length of offspring relative to the length of their parents for each generation during a single run on the lin318 instance. A lower ratio indicates a fitter offspring.

Using an elitist replacement scheme to ensure forward progress, Maximal Sub-Tour Order Crossover performs better than Order Crossover. (See Table 4.1.) In addition to elitism and fitness-based selection, the search procedure for MST-OX also benefits from commonality-based selection. The preservation of common components has improved the performance of a domain-independent (blind) operator.

Table 4.1: Performance of MST-OX and OX on 5 TSP instances. Results are for a steady-state GA with a population size of 1000 run for 250 generations. Values are percent distance from known optimum for average of 5 runs.

TSP Instance	Size	Average Random Start Tour	Avg. Best MST-OX Tour	Avg. Best OX Tour
d198	198	+ 947 %	+ 113 %	+ 85 %
lin318	318	+ 1194 %	+ 301 %	+ 352 %
fl417	417	+ 3723 %	+ 760 %	+ 852 %
pcb442	442	+1328 %	+ 461 %	+ 485 %
u574	574	+ 1627 %	+ 630 %	+ 700 %
average		+ 1764 %	+ 453 %	+ 495 %

4.4 Summary

Crossover operators in genetic algorithms are not completely domain independent. If the manipulated schemata do not match the "structure" of the objective function, fitness-based selection will not amass useful building blocks. For properly matched alleles, the commonality hypothesis helps to identify the most promising building blocks. The preservation of these (common) components allows fitness-based selection to be enhanced by commonality-based selection.

Chapter 5

Heuristic Operators:

Part One

Heuristic operators use problem specific heuristics to generate the (initial) crossover offspring. The Commonality-Based Crossover Framework is the first design model to specifically address this operator category. It suggests that problem specific heuristics should replace (not supplement) the traditional mechanisms of transmission and combination.

5.1 Overview

General methods for function optimization--like genetic algorithms with blind operators--are rarely competitive with problem specific methods. For practical applications, the basic GA mechanisms are often supplemented with problem specific heuristics. If these heuristics (help) select schemata (genes) *during* the crossover process, the resulting procedure is a *heuristic* operator.

The Commonality-Based Crossover Framework defines a two step process for crossover: 1) preserve the maximal common schema of two parents, and 2) complete the solution with a *construction heuristic*. This design model is the first that specifically addresses heuristic operators. In particular, it views the traditional mechanisms as weak heuristics. Specifically, transmission and combination are no longer viewed as the critical features of crossover.

Random recombination does not guarantee that an offspring solution will receive the *best* components from its parents. If the individual components can be independently evaluated, the best components could be (heuristically) combined into an offspring. However, the best components might not be present in the parents. Therefore, the new design model suggests that problem specific heuristics should *replace* (not supplement) combination during the crossover process.

The Commonality-Based Crossover Framework completes a solution with "construction" heuristics--methods that (incrementally) build complete solutions from partial solutions. For the Traveling Salesman Problem, edge-based and order-based construction heuristics are available. With these heuristics, two "commonality-based" heuristic operators have been developed: Common Sub-Tours/Nearest Neighbor (CST/NN) and Maximum Partial Order/Arbitrary Insertion (MPO/AI).

Experiments on CST/NN show that transmission and combination can interfere with the effectiveness of Nearest Neighbor. Experiments on MPO/AI show that an operator's effectiveness improves when the basis of the common schemata matches the basis of the construction heuristic. When these bases are matched, the heuristic operator can handle constraints with the same basis. For example, MPO/AI has been applied to the Sequential Ordering Problem.

5.2 Edge-Based Schemata

The Nearest Neighbor (NN) construction heuristic manipulates edge-based schemata. Starting from a random city, Nearest Neighbor travels to the nearest unvisited city. At each step, the shortest available edge is added to the (partial) solution. After all the cities have been visited, Nearest Neighbor returns to the original start city.

Greedy Crossover [GGR85] is an early heuristic operator that uses Nearest Neighbor to *supplement* (edge) combination. However, the uncommon edges of two Nearest Neighbor parent solutions tend to be the (undesirable) long/crossing edges. (See Figure 3.2.) As a corollary to the commonality hypothesis, uncommon schemata are below average. Therefore, instead of combining these uncommon edges, Nearest Neighbor should generate new edges altogether. Following this advice, Common Sub-Tours/ Nearest Neighbor is developed as a commonality-based heuristic operator. Experimental results show that CST/NN performs better than Greedy Crossover.

5.2.1 Greedy Crossover

It has been suggested that crossover should combine the best genes *from the parents*. With edge-based schemata, this procedure leads to Greedy Crossover (GX). Starting from a random city, GX takes the shortest edge[1] from either parent that connects the current city to an unvisited city. Since transmission and combination are still the primary heuristics, Nearest Neighbor is only used when none of the parent edges are feasible.

The parent edges that are taken may be the good edges responsible for the high observed fitness of the parents, or they may be the poor edges which should be replaced. This lack of differentiation allows poor components to “hitch hike” their way into the offspring by tagging along with the good components. Due to this deficiency, the transmission design principle is a weak (construction) heuristic.

5.2.2 Common Sub-Tours/Nearest Neighbor

The Commonality-Based Crossover Framework suggests that only common edges, which form the Common Sub-Tours (CST), should be taken (preserved) from the parents. By

1. As an influence from Edge Recombination (see section 4.2.2), undirected edges are used instead of directed edges.

the commonality hypothesis, these are the good edges responsible for the high observed fitness of the parents. Treating these common edges/sub-tours as “super nodes”, the normal procedure of Nearest Neighbor can be used. (See Figure 5.1.) The above process defines the Common Sub-Tours/Nearest Neighbor heuristic operator.

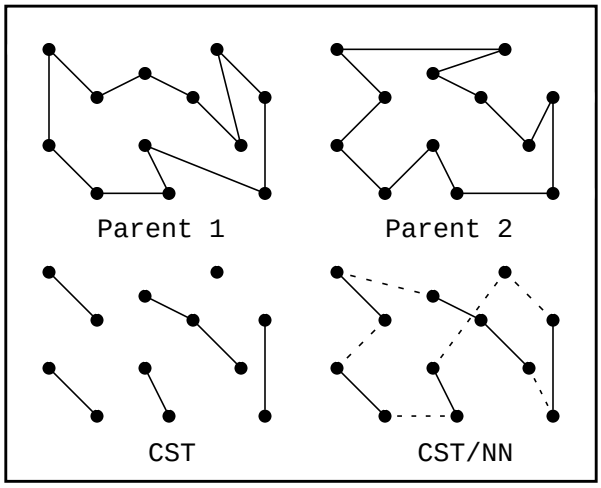


Figure 5.1: Example of CST/NN. The common (CST) edges are preserved, and the remaining uncommon edges are discarded. As a result, there is no opportunity for combination. Instead, Nearest Neighbor is used to generate new edges to complete the offspring solution.

Greedy Crossover and CST/NN both use the Nearest Neighbor construction heuristic. Thus, these experiments isolate the elimination of the transmission design principle from CST/NN. The uncommon components that transmission attempts to preserve are expected to be below average. Thus, changes to these components are more likely to be beneficial--the problem specific heuristic should be more effective than the domain-independent “heuristic”.

5.2.3 Results: CST/NN vs. GX

The Common Sub-Tours/Nearest Neighbor and Greedy Crossover operators have been tested experimentally on a series of TSP instances. The initial population is seeded with Nearest Neighbor started from each city. Since Nearest Neighbor is a deterministic operator, the population is sized to the problem size (to match the number of available start tours). In these experiments, CST/NN finds better solutions than GX. (See Table 5.1.)

Table 5.1: Performance of CST/NN and GX on 5 TSP instances. Results are for a steady-state GA with a population size equal to problem size, run until 20 generations pass without an improvement. Values are percent distance from known optimum for average of 5 runs.

TSP Instance	Avg. Best NN Start Tour	Avg. Best CST/NN Tour	Common Edges From Parents	Avg. Best GX Tour	Common Edges From Parents
d198	+ 12.42 %	+ 5.13 %	100.0 %	+ 10.72 %	99.8 %
lin318	+ 17.06 %	+ 9.16 %	100.0 %	+ 16.95 %	100.0 %
fl417	+ 16.92 %	+ 13.22 %	100.0 %	+ 10.66 %	100.0 %
pcb442	+ 15.17 %	+ 9.64 %	100.0 %	+ 12.11 %	99.0 %
u574	+ 19.92 %	+ 11.36 %	100.0 %	+ 15.98 %	99.9 %
average	+ 16.30 %	+ 9.70 %	100.0 %	+ 13.28 %	99.7 %

Although GX preserves most of the common edges, it also attempts to maximize transmission. Without transmission, CST/NN can explore a larger solution set than GX, and the increase in exploratory power (see section 3.3) leads to a more effective operator. Overall, these experiments suggest that transmission and combination can interfere with the performance of a problem specific heuristic (see chapter 11).

5.3 Order-Based Schemata

Insertion heuristics manipulate order-based schemata. Starting with a partial order of at least three (random) cities, cities are “inserted” into the cyclic partial order between two (currently adjacent) cities. Although this process adds two edges and deletes one edge, order relationships (`1`’s in a Boolean matrix) are only added--city `i` stays before/after city `j` regardless of any additional cities that are inserted between them. At each step, the insertion point is chosen to minimize the incremental increase in distance.

There are no insertion-based heuristic operators available in genetic algorithms, but a comparable procedure exists in A-Teams. For the TSP, a “deconstruction/reconstruction” procedure has used Arbitrary Insertion[1] in the “reconstruction” phase [TdS92]. However, (common) edge-based components are preserved during the “deconstruction” phase, so the two phases manipulate mismatched components. Preserving common order-based schemata instead, Maximum Partial Order/Arbitrary Insertion is developed as a common-

1. At each step, a randomly selected city is inserted.

ality-based heuristic operator. Experimental results show that MPO/AI performs better than the deconstruction/reconstruction procedure.

The MPO/AI operator was originally designed for the TSP. However, it performs better (in relative terms) on the Sequential Ordering Problem (SOP). The SOP is a precedence constrained Hamiltonian path problem. Its order-based constraints can be handled "transparently" by the order-based mechanisms in MPO/AI. Experimentally, MPO/AI found best-known solutions to many SOP instances (although most of these have since been improved by HAS-SOP [GD97]). The results suggest that "transparent" constraints can induce a beneficial search space reduction (see chapter 9).

5.3.1 Deconstruction/Reconstruction

As defined in A-Teams[TdS92], the goal of deconstruction is to identify useful components (e.g. building blocks) in existing solutions. Ideally, better solutions can be reconstructed from these components. The following deconstruction mechanism identifies the common edges of two parents. However, they are not used as edges--they are used to create a partial order by dropping the remaining cities from Parent 1. (See Figure 5.2.)

```
Parent 1:  a b c d e f g h i j k l
Parent 2:  a c d e k i j f h g l b

common
edges :    a-b   d-e   g-h   i-j

partial
order :    a b d e g h i j
```

Figure 5.2: Example of deconstruction. Although common edges are preserved, their orientation can be reversed between parents (e.g. a-b and g-h).

Arbitrary Insertion performs reconstruction by rebuilding a complete solution from the partial order. Unfortunately, the initially preserved common edges can be deleted during insertion. Since the common parent components (edges) are not always preserved in the final offspring solution, deconstruction/reconstruction does not necessarily benefit from commonality-based selection.

5.3.2 Maximum Partial Order/Arbitrary Insertion

The neighborhood considered by deconstruction/reconstruction does not always include both parents. Specifically, if any of the common (undirected) edges have reverse (directed) orientations, then insertion cannot rebuild Parent 2 from the partial order. Since a common schema is a partial order that insertion can extend into both parents, the schemata identified by deconstruction may not be common to both parents. The longest common partial order is the Maximum Partial Order (MPO). Using Arbitrary Insertion to complete this partial solution, the overall process defines the Maximum Partial Order/ Arbitrary Insertion heuristic operator.

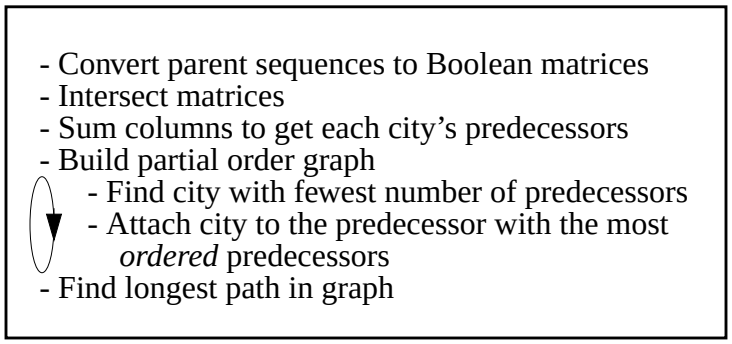


Figure 5.3: Pseudo-code to find the Maximum Partial Order of two parent sequences.

The pseudo-code for generating the Maximum Partial Order of two parents is listed in Figure 5.3. To convert the parent sequences into Boolean matrices, all solutions are assigned the same start city and the same orientation[1]. Since element `(i, j) = 1` when city `i` precedes city `j` in the sequence, the intersection matrix has element `(i, j) = 1` if and only if city `i` precedes city `j` in both parents. These `1`'s represent the common order-based schemata of two parents.

1. Three evenly spaced convex hull cities (e.g. `a`, `b`, `c`) define the orientation of all solutions (i.e. `a...b...c...`). These cities are the start cities for the three segments that compose the MPO (i.e. the MPO procedure is run three times during MPO/AI).

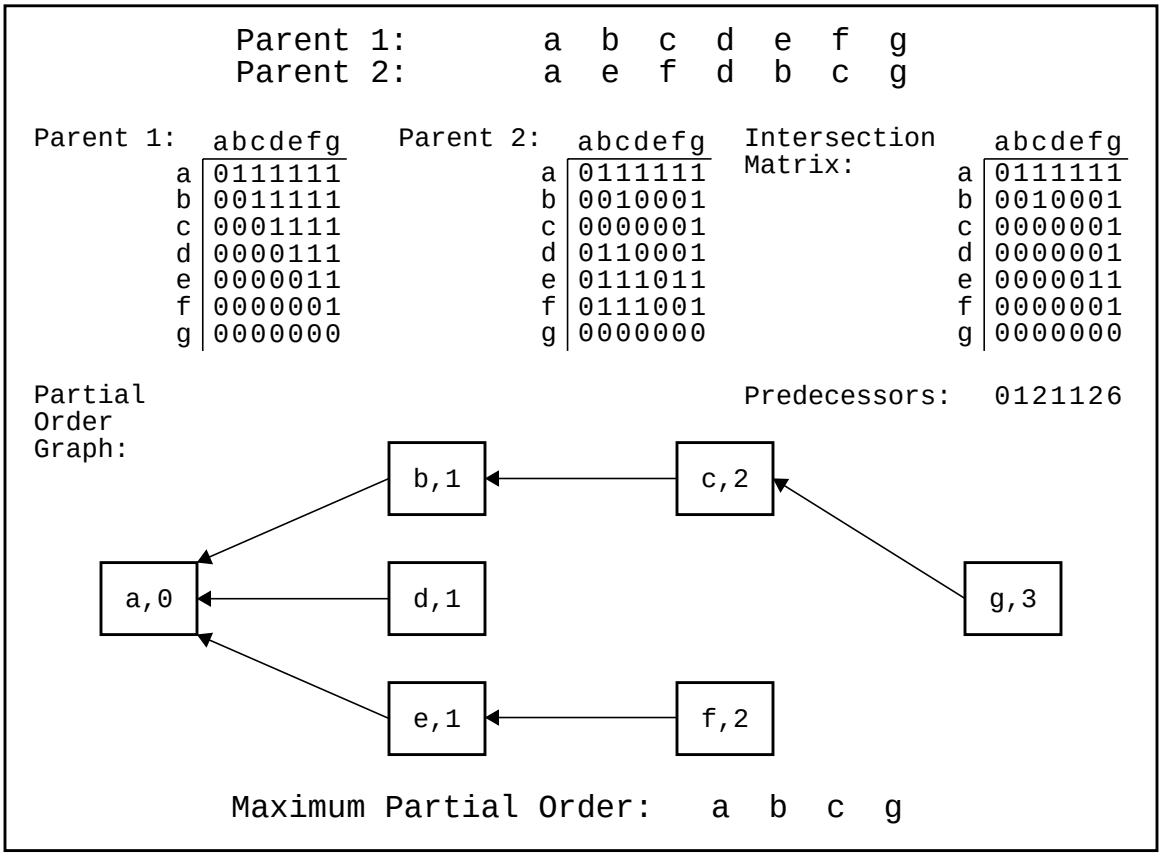


Figure 5.4: Example of MPO. City `a` is the segment start city, so it has `0` ordered predecessors at the root of the partial order graph. City `g` is preceded by all of the cities in the graph, but it can only be attached to cities `c` and `f` because those cities have the most ordered predecessors (`2`).

In the intersection matrix, the column sums give the number of common predecessors for each city. Using the segment start city as the root of the partial order graph, cities are added in increasing order of their predecessors[1]. Each city is "attached" to the common predecessor (identified by a `1` in its column of the intersection matrix) with the most "ordered" predecessors. The new city will have one more ordered predecessor than the city it is attached to--each node represents the longest partial order for that city. When all cities have been added, the longest path represents the Maximum Partial Order. (See Figure 5.4.)

1. All ties are broken randomly.

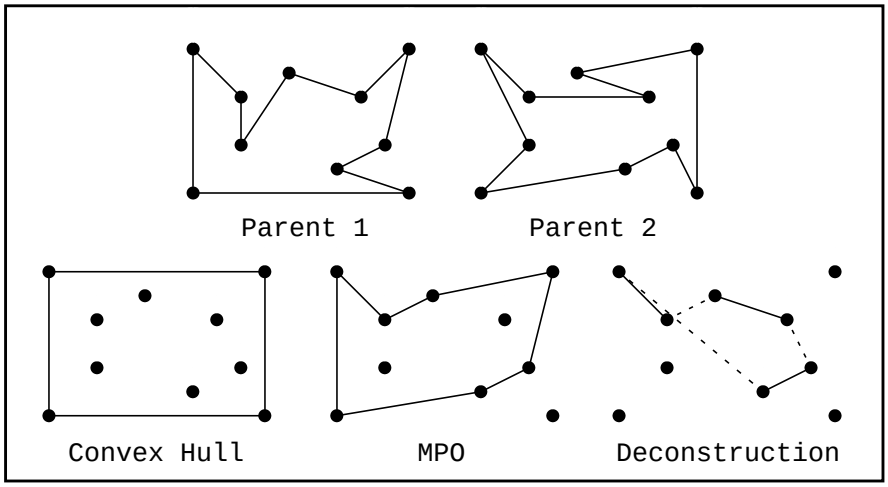


Figure 5.5: Example of "shape" from the convex hull, the MPO, and deconstruction.

As order-based schemata, partial orders represent "shape" templates. Shape is useful (for geometric TSPs) because insertion heuristics perform better when they are started from good "outlines". For example, if AI is started with the convex hull, it will find solutions about 1% better than those found with three random cities [Rei94]. The shape of the MPO is more refined than the convex hull (see Figure 5.5), so AI should perform even better when it is (re)started from this partial solution.

5.3.3 Results: MPO/AI vs. Deconstruction/Reconstruction

The MPO/AI operator and the deconstruction/reconstruction procedure have been tested experimentally on a series of TSP instances. The initial population is seeded with 400 Arbitrary Insertion solutions each started from the convex hull. To reduce the rate of convergence with MPO/AI, one parent is chosen randomly. In these experiments, MPO/AI performs better than deconstruction/reconstruction. (See Table 5.2.)

Table 5.2: Performance of MPO/AI and deconstruction/reconstruction on 5 TSP instances. Results are for a steady-state GA with a population of 400 run until 10 generations pass without an improvement. Values are percent distance from known optimum for average of 5 runs. Experiment runtimes are given for a SPARC 20.

TSP Instance	Average Best Convex Hull/ AI Start	Average Best MPO/AI	Runtime (min)	Average Best Deconstruction/ Reconstruction	Runtime (min)
d198	+ 3.05 %	+ 0.95 %	3	+ 1.31 %	1
lin318	+ 6.04 %	+ 0.63 %	13	+ 3.38 %	2
fl417	+ 1.91 %	+ 0.57 %	15	+ 0.52 %	7
pcb442	+ 8.97 %	+ 1.84 %	37	+ 4.20 %	9
u574	+ 8.45 %	+ 2.20 %	74	+ 4.01 %	13
average	+ 5.68 %	+ 1.24 %		+ 2.68 %	

Deconstruction uses the natural (symbolic) representation for TSP solutions, so it is much faster than finding the MPO--which has an $O(n^2)$ time complexity. However, the partial order of deconstruction is not as useful as the Maximum Partial Order. The outline produced from (common) edges might not represent the “shape” (defining schema) of two parent solutions. (See Figure 5.5.)

5.3.4 MPO/AI and the Sequential Ordering Problem

The Sequential Ordering Problem (SOP) is a constrained Hamiltonian path problem. Specifically, $d(c_i, c_j) = -1$ represents a precedence constraint that requires node j to precede (not necessarily immediately) node i in the sequence[1]. The objective is to find the shortest Hamiltonian path through the graph of n nodes subject to satisfying the precedence constraints. Visually, if a courier has n clients to visit, and clients with objects to be “picked up” must be visited before those objects can be “dropped off”, find a sequence such that travel distance is minimized--subject to visiting each client once and only once and performing all (paired) pick-ups before their corresponding drop-offs. Formally, given n nodes c_i with edge weights $d(c_i, c_j)$, find a sequence π of the n nodes such that the following sum is minimized and all precedence constraints are satisfied:

1. For convenience, problem matrices tend to include “dummy” nodes for the first and last positions of the (non-cyclic) sequence.

$$\min_{\pi} \sum_{k=1}^{n-1} d(c_{\pi(k)}, c_{\pi(k+1)})$$

if $d(c_i, c_j) = -1$

then $l < k$

for $\pi(l) = j$, $\pi(k) = i$

Although the objective of the SOP is edge-based, its constraints are order-based--$d(c_i, c_j) = -1$ requires node j to precede node i, but it does not constrain the number of (*inserted*) nodes between them. Therefore, the constraints are transparent to insertion. Further, the intersection matrix of two feasible parents includes all of their (satisfied) precedence constraints--each constraint specifies a 1 in the Boolean matrix. Subsequently, MPO/AI can be applied to the Sequential Ordering Problem with minor modifications[1].

The MPO/AI operator has been tested experimentally on a series of SOP instances[2]. The initial population is seeded with 500 Arbitrary Insertion solutions. In these experiments, MPO/AI finds new best-known solutions for many of the tested SOP instances. Although MPO/AI is slowed by the $O(n^2)$ time complexity associated with matrix representations, it is still faster than a branch and cut algorithm[3] [Asc96]. MPO/AI uses roughly 2% of the computational effort to reach the (best-known solution) bounds set by the branch and cut algorithm. (See Table 5.3.)

The order-based mechanisms of MPO/AI match the order-based constraints of the SOP. This transparently reduces the search space--MPO and AI are oblivious to the existence of the precedence constraints. In contrast, order-based constraints create “obstacles” in edge-based search spaces. Thus, edge-based methods (e.g. integer programming) require additional mechanisms to handle the constraints explicitly. If these mechanisms interfere with the process of optimization, relative performance can suffer. Although branch and

1. AI is modified to generate only feasible solutions, and MPO is modified to use only one segment.
2. These instances are also taken from TSPLIB (see section 2.9.2).
3. In this study, the branch and cut algorithm was run for 300 minutes on a SPARC 2; 1200 minutes for the larger “rbg” instances.

cut algorithms can find optimal solutions on the TSP, they are less effective (than MPO/AI) on the SOP.

Table 5.3: Performance of MPO/AI on 16 SOP instances taken from TSPLIB. Results are for 5 runs of a steady-state GA with a population of 500 run until 20 generations pass without an improvement. Overall best MPO/AI solutions in bold improved the previous best-known bounds. (Asterisks indicate that bound is still current.) Times are given for execution on a SPARC Ultra 1 (167 MHz).

SOP Instance	Size	Con-straints	Average Best AI Start	Average Best MPO/AI	Overall Best MPO/AI	Original Branch and Cut Bounds [Asc96]	Time to Bound (s)	Runtime (s)
ft70.1	71	17	41809	39615	39545	**39313**	NA	76
ft70.2	71	35	43485	40435	**40422**	[39739, 41778]	5.4	73
ft70.3	71	68	46731	42558	*** 42535**	[41305, 44732]	2.8	48
ft70.4	71	86	55982	53583	**53562**	[52269, 53882]	2.4	47
kro124p.1	101	25	45758	40996	**40186**	[37722, 42845]	5.4	136
kro124p.2	101	49	49056	42576	**41677**	[38534, 45848]	5.2	94
kro124p.3	101	97	63768	51085	**50876**	[40967, 55649]	3.8	103
kro124p.4	101	131	87975	76103	*** 76103**	[64858, 80753]	2.0	76
rbg323a	325	2412	3466	3161	**3157**	[3136, 3221]	207.6	1566
rbg341a	343	2542	3184	2603	**2597**	[2543, 2854]	70.6	2205
rbg358a	360	3239	3165	2636	**2599**	[2518, 2758]	533.8	4491
rbg378a	380	3069	3420	2843	**2833**	[2761, 3142]	67.6	5354
ry48p.1	49	11	16602	15813	*** 15805**	[15220, 15935]	2.4	22
ry48p.2	49	23	18071	16676	*** 16666**	[15524, 17071]	1.6	32
ry48p.3	49	42	22074	19905	*** 19894**	[18156, 20051]	7.6	29
ry48p.4	49	58	32591	31446	31446	[29967, 31446]	5.0	19

5.4 Additional Comments

As indicated by the lack of asterisks, new best-known solutions have since been found for many of the presented SOP instances. These solutions were found by HAS-SOP: a Hybrid Ant System for the Sequential Ordering Problem [GD97]. In HAS-SOP, an initial solution (of unreported quality) is generated by an ant colony (see section 2.8.5), and it is locally optimized with a “lexicographic” search operator. Essentially, a hybrid operator has been compared to a heuristic operator. The new distinction between heuristic and hybrid operators leads to better (more direct) comparisons among operator instances.

When the lexicographic operator is added to MPO/AI, the performance improvement does not match HAS-SOP. The ant colony appears to have two advantages over MPO/AI for generating initial solutions. First, the ant colony uses a natural representation, so it is much faster. Second, the ant colony appears to maintain better diversity. The strict preservation of common components in MPO/AI can cause undesirably strong convergence effects. These advantages are less easily observed when HAS-SOP is compared directly to MPO/AI.

5.5 Summary

The Commonality-Based Crossover Framework is the first design model to specifically address the category of heuristic operators. Using the same (traditional) construction heuristic as previous operators, the superior performance of the new operators isolates the role of preserving common components. Further, these results suggest two key extensions. First, the results of CST/NN suggest that the transmission design principle can handicap the effectiveness of a problem specific heuristic (see chapter 11). Second, the results of MPO/AI suggest that beneficial search space reductions can be developed for commonality-based operators (see chapter 9).

Chapter 6

Heuristic Operators:

Part Two

As the primary focus of the Commonality-Based Crossover Framework, heuristic operators deserve a deeper examination. This analysis leads to commonality-based selection, heuristic amplification, and open-loop optimization.

6.1 Overview

The first step in the new design model states, “preserve the maximal common schema of two parents”. This directive causes common schemata to be *selected*. To isolate this commonality-based form of selection, GENIE (a GA without fitness-based selection) is developed. When heuristic operators are implemented in GENIE, the (additional) selective pressure supplied through commonality-based restarts can be observed. The existence of commonality-based selection corroborates the commonality hypothesis--the preserved common schemata are above average.

The commonality hypothesis provides a “confidence measure” on the performance of construction heuristics--common decisions should be correct. Thus, heuristic operators can use commonality-based selection to identify highly-fit partial solutions. With this accumulated knowledge, restarts can develop better solutions. This effect represents *heuristic amplification*.

The Schema Theorem suggests that global payoff information is *sufficient* to perform optimization. However, the existence of heuristic amplification suggests that it is no longer *necessary.* If a standard genetic algorithms performs black box optimization (no problem model is required), then a heuristic operator in GENIE is analogous to open-loop optimization (no fitness feedback is required at the level of complete individuals).

6.2 GENIE

In the analysis of ideal construction heuristics (see section 3.7.2), the proportion of correct schemata was calculated for each generation of a GA with random parent selection and generational replacement. These features define GENIE--a GA that selects neither mating parents nor surviving offspring on the basis of their fitness[1]. With the elimination of fitness-based selection at the individual, GENIE allows commonality-based selection to be isolated[2].

1. Note: all parents mate twice during each generation to help reduce random biases.
2. For GENIE with finite populations, drift effects are still present.

6.3 Heuristic Amplification

To amplify the effectiveness of construction heuristics, partial solutions with high proportions of fit schemata are required (see section 3.7). Common schemata (i.e. the schemata chosen by commonality-based selection) can form these desirable partial solutions. Therefore, it should be more effective to embed a construction heuristic into a commonality-based operator than to use random restarts.

An ideal construction heuristic and a commonality-based heuristic operator have been developed for One Max. In experiments, it is shown that common schemata are fitter than random/average schemata (of the parents). Restarts from these partial solutions are more effective--the (ideal) heuristic operator exhibits heuristic amplification.

The CST/NN and MPO/AI heuristic operators have also been implemented in GENIE. Experimental results demonstrate that heuristic amplification can occur in practical operators--even though non-ideal characteristics exist (e.g. "negative" heuristic amplification). To combat the effects of negative heuristic amplification, fitness-based selection (of parents) can be applied.

6.3.1 One Max

The correct gene for each allele is a `1`. Therefore, a trivial heuristic for One Max is to select more `1`'s than `0`'s. For example, select a `1` for each allele with a (constant) probability of $p = 0.6$, and a `0` with a probability of $1 - p = 0.4$. This (construction) heuristic is ideal because the decision at each step has a constant (and independent) probability of being correct.

The above heuristic has been embedded into a commonality-based heuristic operator and implemented in GENIE. For a One Max problem of 100 bits, GENIE is run for 20 generations with a population size of 100. Starting from an initial population that is seeded by random restarts of the construction heuristic, the optimal solution is always found. (See Table 6.1.) The superior fitness of the final solutions demonstrates that heuristic amplification has occurred.

Table 6.1: Results for an ideal construction heuristic in GENIE.

	Avg. Best Start	Avg. Best Overall
One Max	72.1	100.0

To measure the effects of commonality-based selection, the average fitness of the partial solutions has been recorded. The ratio of `1`'s to `0`'s in the common schemata is always greater than the corresponding ratio for random schemata in the entire population. (See Figure 6.1.) The commonality hypothesis is valid in this experiment--the average fitness of the common components was above the average fitness of their parents.

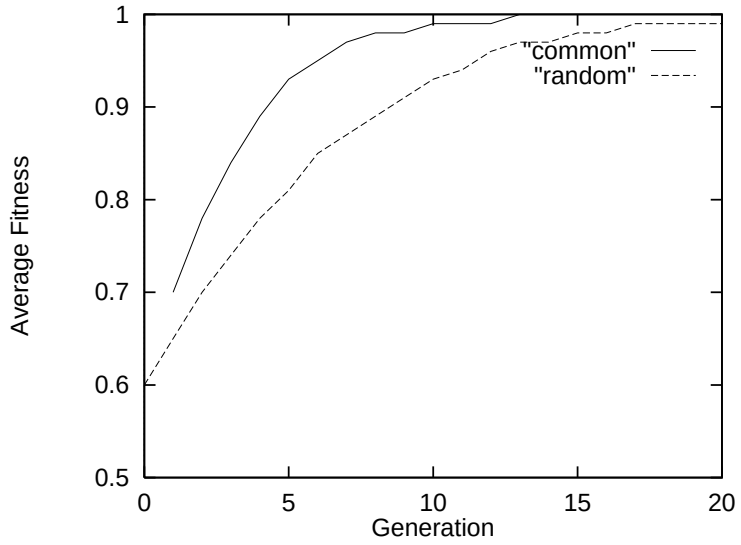


Figure 6.1: Average fitness of common and random components in One Max.

Since common components are above average, the average fitness of the remaining uncommon components must be below the average fitness of the parents. In particular, an uncommon allele will have a `1` in one parent and a `0` in the other. The average fitness of uncommon components in One Max is always 0.5.

6.3.2 Common Sub-Tours/Nearest Neighbor

A practical construction heuristic (e.g. Nearest Neighbor) is not expected to make correct decisions with a constant probability. For example, constraints may disallow the correct decision at any given step. Nonetheless, to study the effects of heuristic amplification for practical construction heuristics, Common Sub-Tours/Nearest Neighbor has been implemented in GENIE.

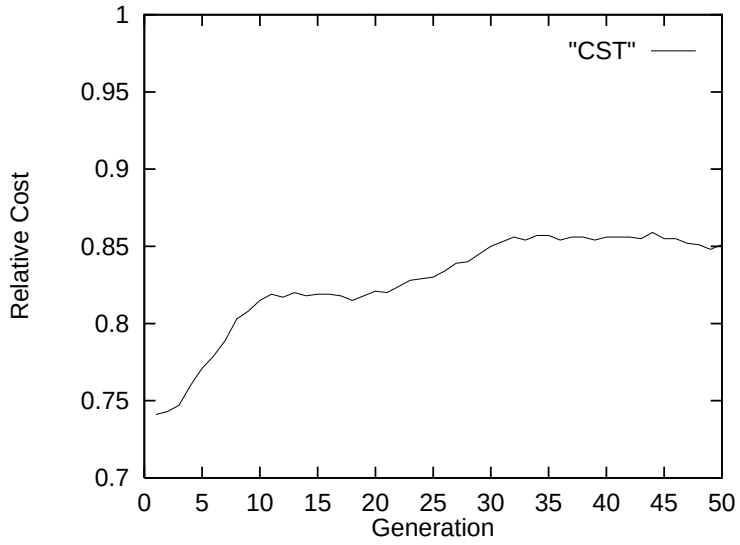


Figure 6.2: Relative cost of common (CST) edges in CST/NN for a single run on the lin318 instance.

The common (CST) edges of two parents should be their short edges. (See Figure 3.2.) This expectation is confirmed by measuring their relative fitness (relative cost)--the common edges are much shorter than average. (See Figure 6.2.) However, even with these promising partial solutions, the results for CST/NN are unimpressive. (See Table 6.2.) Since only 14% of the initial surplus from optimal is reduced from the best start solutions to the best final solutions, almost no heuristic amplification has occurred.

Table 6.2: Results for CST/NN in GENIE. Population size is equal to problem size. Initial population is Nearest Neighbor started from each city. Values are percent surplus from known optimum for average of 5 runs (50 generations each).

TSPLIB Instance	Avg. Best NN Start Tour	Avg. Best CST/NN Tour
d198	+ 12.42 %	+ 8.67 %
lin318	+ 17.06 %	+ 16.30 %
fl417	+ 16.92 %	+ 13.37 %
pcb442	+ 15.17 %	+ 13.30 %
u574	+ 19.92 %	+ 18.40 %
average	+ 16.30 %	+ 14.01 %

For the TSP, it is not just the number of correct/incorrect edges that determines solution quality. The length (relative fitness) of the incorrect edges (schemata) is also important. Further, starting with a partial solution of short edges does not necessarily reduce the tendency of Nearest Neighbor to “paint itself into a corner”. These results suggest that Nearest Neighbor is a poor heuristic (very far from ideal).

6.3.3 Maximum Partial Order/Arbitrary Insertion

Maximum Partial Order/Arbitrary Insertion has also been implemented in GENIE. Since a partial order represents an exponentially large number of solutions, the fitness of the MPO cannot be measured directly. Nonetheless, it appears to have a superior relative fitness--MPO/AI in GENIE reduces the surplus from optimal by 66% from the best start solutions to the best final solutions. (See Table 6.3.)

Table 6.3: Results for MPO/AI in GENIE. Population size is 400, and the initial population is 400 AI solutions started from the convex hull. Values are percent surplus from known optimum for average of 5 runs (50 generations each).

TSPLIB Instance	Avg. Best Convex Hull/AI Start Tour	Avg. Best MPO/AI Tour
d198	+ 3.05 %	+ 1.24 %
lin318	+ 6.04 %	+ 1.75 %
fl417	+ 1.91 %	+ 0.58 %
pcb442	+ 8.97 %	+ 3.48 %
u574	+ 8.45 %	+ 2.59 %
average	+ 5.68 %	+ 1.93 %

The fitness of a partial order can be estimated by a random sample of the solutions that it represents. For measurement convenience, the average fitness of a population is used to approximate the fitness of common schemata in mating parents. This average fitness has been measured for a single run of MPO/AI on the lin318 instance. (See Figure 6.3.)

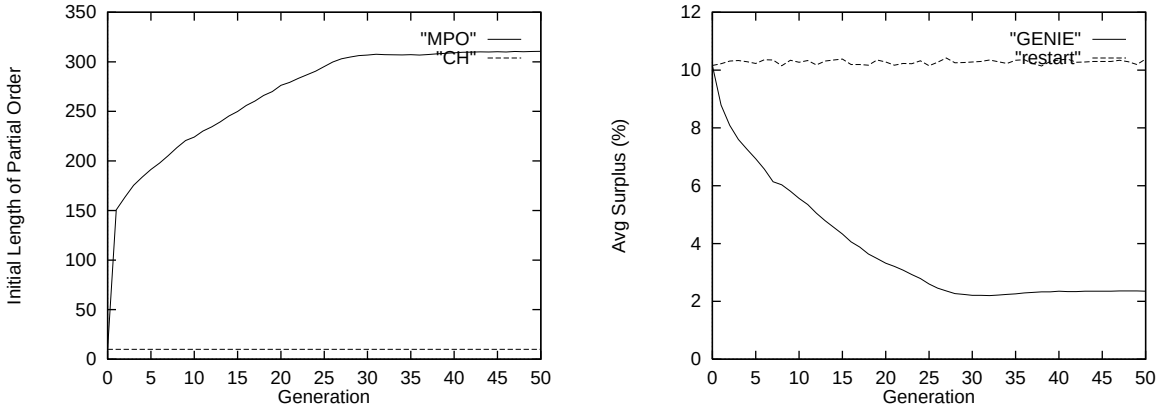


Figure 6.3: Average population fitness (surplus) for MPO/AI in GENIE and (random) convex hull restarts of Arbitrary Insertion. Fitter populations imply fitter initial schemata. Thus, the MPO is fitter than the convex hull.

In addition to average fitness, the average length of the MPO for mating parents was also recorded. The size of the partial solution preserved by commonality-based selection grows consistently through generation 27. Further, the average quality of the MPO/AI solutions also improves steadily until generation 28. After this phase of convergent search, a "drift" phase begins which appears to degrade solution quality.

To baseline the MPO/AI results, 50 generations of Arbitrary Insertion restarts from the convex hull are also plotted. The convex hull (CH) is a static entity, so it does not accumulate information from previous solutions. Without information accumulation, there is no "persistence ratchet" [Sha99] to advance search. Compared to the solution quality of random restart which does not improve over time, these results demonstrate that commonality-based selection has supplied selective pressure--it has identified and preserved partial orders of increasing fitness and specificity.

6.3.4 Negative Heuristic Amplification

The effects of heuristic amplification can also be bad. If the probability of making incorrect decisions is greater than the probability of making correct decisions, then incorrect schemata will eventually dominate the population. For MPO/AI, its worst performance occurs on the pcb442 instance. The "structure" of this instance induces Arbitrary Insertion to make incorrect decisions that are non-random and non-independent. (See Figure 6.4.)

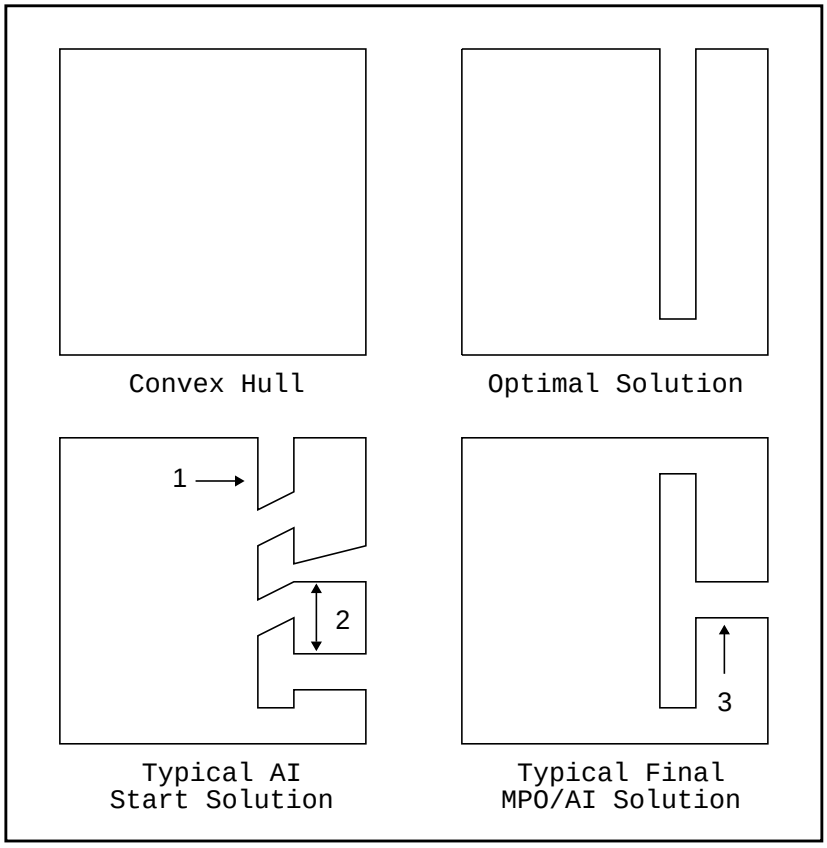


Figure 6.4: Simplified outlines of several pcb442 solutions.

The optimal solution for the pcb442 instance includes a “shaft”. To traverse this shaft correctly, cities must be inserted (in order) from the top. Otherwise, the inserted cities may be incorrectly attached to the “right” edge. Since the next city is chosen randomly, there are *fewer* correct decisions (see pointer 1) than incorrect decisions (see pointer 2). As systematic errors, these incorrect decisions are likely common to all parents. Negative heuristic amplification subsequently causes the final solution to be defined by these incorrect decisions (see pointer 3).

6.3.5 Heuristic Amplification and Fitness-Based Selection

Examining the results for CST/NN (see Table 6.2 and Table 5.1) and the results for MPO/AI (see Table 6.3 and Table 5.2), the performance of heuristic operators improves when fitness-based selection is used. Fitness-based selection provides an additional confidence measure on the performance of a construction heuristic. In particular, fitness-based selection can help counteract the effects of negative heuristic amplification.

For example, the ideal construction heuristic for One Max (see section 6.3.1) has been redesigned to select `1`'s with a probability of `p = 0.45`. Since this heuristic makes incorrect decisions more often than correct decisions, the resulting heuristic operator is prone to negative heuristic amplification. This operator has been implemented in GAs with (GENITOR) and without (GENIE) fitness-based selection. On a problem of 100 bits with a population size of 100 solutions, GENITOR goes forward while GENIE goes backward. (See Figure 6.5.)

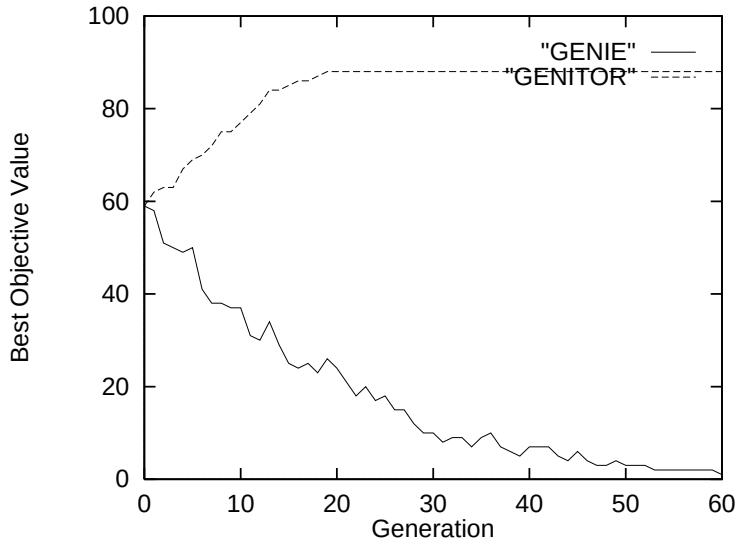


Figure 6.5: Sample result for GENIE and GENITOR when `p = 0.45`.

Commonality-based selection is weak when the construction heuristic is weak. Since practical (non-ideal) heuristics will have areas of weakness, fitness-based selection should still be useful. Although commonality-based selection can enhance fitness-based selection, it does not replace it.

6.4 Open-Loop Optimization

Closed-loop control is favored over open-loop control. However, feedback is not always available (or useful). For example, rocket launches are open-loop--by the time the launch vehicle is observed to be off course, it is too late. Likewise, it appears that fitness-based selection (used in closed-loop optimization) can always improve the performance of

heuristic operators (see section 6.3.5). Nonetheless, open-loop optimization is presented as an available method.

Open-loop optimization is the reverse of black box optimization. In black box optimization, the structure of the problem is not modeled, but the fitness must be observable. Genetic algorithms can then use domain-independent operators and fitness-based selection at the individual level. Conversely, if the problem structure can be modeled with enough accuracy, global payoff information may not be necessary. Specifically, heuristic operators and commonality-based selection can be used instead. For both cases, the overall objective must be decomposable--good solutions consist of good schemata, and good schemata form good solutions.

In the experiments with MPO/AI in GENIE (see section 6.3.3), the fittest solutions are often found in the last generation of the "convergent search" phase (when the average MPO of mating parents is increasing monotonically). If GENIE is stopped when the amount of schemata common to mating parents does not increase for the first time, the best solution should be present in the final population. Further, this solution should be optimal for an ideal construction heuristic (see section 3.7.2). Since intermediate solutions do not need to be evaluated, open-loop optimization (non-fitness-based evolution) can be pursued.

The results for heuristic operators in GENIE (see section 6.3) can be trivially converted into results for open-loop optimization. Thus, this section focuses on finding optimal solutions. Although the entire population should converge to the optimal solution for an ideal construction heuristic, the same is not expected for practical heuristics.

6.4.1 One Max

Using `p = 0.6`, the ideal heuristic operator for One Max has been implemented in GENIE. For a problem with 100 bits, a population size of 100 is used. When the commonality-based stop condition is reached (i.e. when the number of bits common to mating parents fails to increase), a *single* (randomly chosen) member of the final population is evaluated. In 30 trials, this solution was optimal 25 times. (See Table 6.4.)

Table 6.4: Ideal construction heuristic in GENIE versus restarts.

Method	Optimal Trials	Average Best
GENIE	25/30	99.8
3000 Restarts	0/30	77.4

6.4.2 Maximum Partial Order/Arbitrary Insertion

Since no optimal solutions were found in the previous experiments with MPO/AI (see section 6.3.3), these experiments use the (easier) kroA100 instance. A population size of 100 is used, and GENIE is initialized with 100 solutions of Arbitrary Insertion started from the convex hull. The average length of the MPO in mating pairs is recorded for each generation, and GENIE is stopped when the average MPO does not increase for the first time. All of the solutions in the final population are then evaluated.

In 30 trials, convergence requires an average of 8 generations, the average length of the MPO at convergence is 90 cities, and the optimal solution is found 18 times. (See Table 6.5.) For comparison, 1000 random restart (seed) solutions of Convex Hull/Arbitrary Insertion (CH/AI) are also run. In 30 trials, random restarts never finds the optimal solution.

Table 6.5: MPO/AI in GENIE on kroA100 versus 1000 random CH/AI solutions.

Operator Algorithm	Optimal Trials	Average Best (% surplus)
MPO/AI GENIE	18/30	+ 0.04 %
CH/AI 1000 restarts	0/30	+ 0.44 %

The schemata in the convex hull are correct--they are part of the optimal solution [Rei94]. The additional cities in the MPO must also be largely correct since optimal solutions were found. Therefore, commonality-based selection can identify correct schemata, and open-loop optimization with non-ideal operators is feasible.

6.5 Summary

The GENIE algorithm allows the effects of commonality-based selection to be isolated in heuristic operators. With the elimination of fitness-based selection, (positive) heuristic amplification and open-loop optimization depend upon the selective pressure supplied by commonality-based restarts. Since the preserved common components must be above average to observe these effects, their existence depends on a satisfied commonality hypothesis. In the preceding experiments, the common schemata preserved from the above-average (parent) solutions were indeed above average.

Chapter 7

Hybrid Operators

A hybrid operator uses a local optimizer to post-process an initial start solution. The quality of this solution affects the efficiency and effectiveness of the overall hybrid operator. Compared to other forms of crossover, commonality-based heuristic operators may provide better restart points.

7.1 Overview

A crossover operator and a local optimizer form a *hybrid operator.* Since crossover operators (heuristic or domain-independent) rarely produce locally optimal solutions, the offspring can be improved by a local optimizer (i.e. hill climbing procedure). Unlike heuristic operators which incorporate problem specific knowledge into the crossover process, hybrid operators apply local search procedures *after* crossover[1].

In a "hybrid GA"[2], crossover produces start points. However, the goal of finding good solutions is different from the goal of finding good start points. Therefore, operators that have been designed as independent entities are unlikely to be effective restart methods. The crossover operator should be matched to the local optimizer.

Despite the lack of intentional synergy, the two stages of a hybrid operator can still cooperate. For example, local optimizers provide crossover operators with better building blocks to combine. Conversely, (fitter) crossover offspring reduce the computational effort expended by local optimizers to bring random start solutions into the near-optimal region [UPL91]. In general, hybrid GAs are more effective than random restarts of the local optimizer.

Although better than a random restart, the behavior of a weak, poorly matched, or otherwise poorly designed crossover operator may not be significantly different. If crossover does not consider the neighborhood structure of the local optimizer, the provided offspring solution can exceed the exploratory horizon (of the parents). When there is little correlation between the fitness of the parents and offspring, the search procedure is effectively random. Therefore, crossover design affects the performance of the overall hybrid operator.

The Commonality-Based Crossover Framework focuses on two aspects. First, if the initial offspring solution is fitter, the computational efficiency of the local optimizer can increase. Second, by exploiting common components which match the (neighborhood) structure of the objective, the final offspring solutions should be less distant from their

1. This distinction between heuristic and hybrid operators is newly introduced. Previously, these terms have been used interchangeably.
2. These have also been called memetic algorithms [RS94].

(above-average) parents. In a globally convex search space (like the TSP), offspring that are closer to their parents will often be fitter.

7.2 Globally Convex Search Spaces

It has been suggested that hybrid GAs should be analyzed as best-of-k-runs approaches [JM97]. If the local optimizer is solely responsible for the overall effectiveness of the hybrid operator, then the perspective of neighborhood search is irrelevant. However, local optima are often "clustered" in the search space (i.e. local optima have a neighborhood structure). Therefore, neighborhood search is still relevant because good (locally optimal) solutions can be used to find others.

When local optima are clustered in a "big valley", the search space is *globally convex*. The existence of this structure causes locally optimal solutions to be closer to (have more in common with) each other than random solutions [Müh91][Boe96][MBK97]. Conversely, meta-heuristics (e.g. genetic algorithms, tabu search, etc) are not useful without this structure. Random restart should be equally effective when good solutions are randomly distributed.

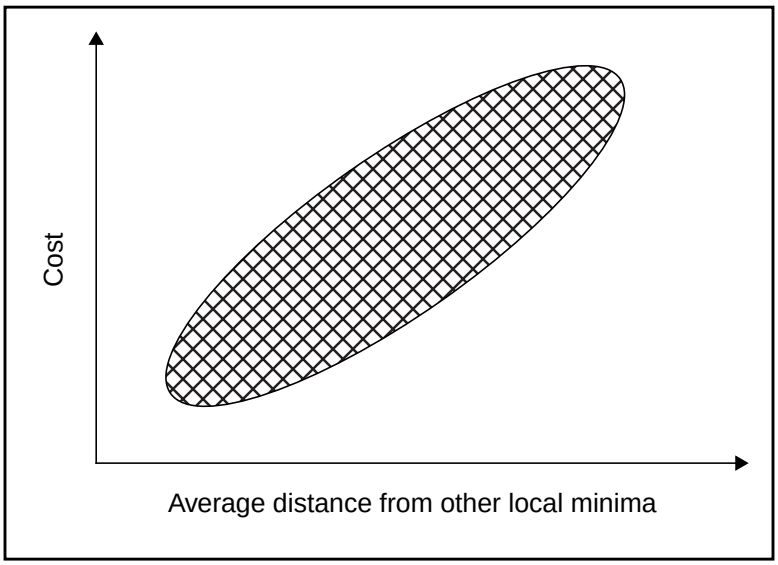


Figure 7.1: Typical distribution of local optima for the TSP.

Scatter plots are the best tool to observe the big valley structure of the TSP. When generating these graphs, each point represents a random local optima--fitness is on the y-axis

and average distance is on the x-axis[1]. In a typical scatter plot, the (2500) points fill a diagonal ellipsoid [Boe96]. (See Figure 7.1.) The best solutions (in the lower left corner) are closest to the other local optima--they are in the center of the big valley!

- Generate an initial population of random local optima
- Generate new local optima from adaptive starting tours

Figure 7.2: Simplified outline for Adaptive Multi-Start.

To explore this big valley, an Adaptive Multi-Start (AMS) procedure has been proposed [Boe96]. (See Figure 7.2.) This procedure is similar to a hybrid GA that uses a multi-parent, domain-independent operator to generate start points[2]. (See Figure 7.3.) Although this construction procedure targets the common components that define the big valley, it does not explicitly exploit its *structure*.

- Create a set of edges from selected parents
- Weight edges based on parent fitness
- Add edges to “offspring” solution in order of weights
- Add feasible edges as required to complete solution

Figure 7.3: Simplified outline to construct adaptive starting tours for AMS.

The results for Adaptive Multi-Start are not significantly better than random restart[3]. Since the analysis of AMS focuses on the population aspects (i.e. selection and replacement), the role of the (implicit) hybrid operator is less thoroughly examined. The following experiment on hybrid operators identifies weaknesses in the (domain-independent) model for adaptive starting tours.

1. For the TSP, the (Hamming) distance represents the number of different edges between two solutions.
2. This procedure can be viewed as a multi-parent form of Edge Recombination (see section 4.2.2).
3. See Table 8.2 in [Boe96].

7.3 Hybrid Operators for the Traveling Salesman Problem

Three hybrid operators that use 2-opt as the local optimizer are examined for the Traveling Salesman Problem. Since the 2-opt local optimizer is held constant, these experiments isolate the role of crossover. It is shown that offspring solutions with high individual fitness can (synergistically) reduce the work load of the local optimizer. Subsequently, the search effort is focused into a small (promising) neighborhood that surrounds the two parent solutions.

7.3.1 The Local Optimizer

The 2-opt local optimizer is an edge-based hill climbing procedure. In a TSP solution, each pair of edges can be exchanged for another pair of edges that will feasibly connect the same four cities. If the alternative edge pair is shorter than the current edge pair, the exchange is executed[1]. This procedure uses the smallest possible neighborhood size--it disrupts the fewest edges.

7.3.2 The Crossover Operators

The three hybrid operators are extended from a commonality-based heuristic operator, a heuristic operator that uses combination, and a domain-independent operator. Since the basis of the 2-opt local optimizer is edges, these crossover operators are all based on edges as well. The operators are Common Sub-Tours/Nearest Neighbors (see section 5.2.2), Greedy Crossover (see section 5.2.1), and Random, Respectful Recombination [Rad91].

Random, Respectful Recombination (RRR) first preserves the common edges, and then it selects the remaining edges randomly. In general, RRR is weaker than Edge Recombination because random edges are less fit than parent edges (which fitness-based selection has evaluated indirectly). However, hybrid operators with RRR have been previously reported [Esh91], and RRR is sufficient to demonstrate the weaknesses of the (domain-independent) adaptive starting tours in AMS.

1. The “random” hill climbing version of 2-opt is used. Whenever an improving exchange is found during a sequential scan of all edge pairs, it is taken.

7.3.3 The Hybrid Operators

Greedy Crossover solutions often have crossing edges that 2-opt can correct. Thus, 2-opt has been appended to form the GX-2-opt hybrid operator [SG87]. Since CST/NN solutions also have crossing edges, 2-opt is again appended to form the CST/NN-2-opt commonality-based hybrid operator. (See Figure 7.4.) These hybrid operators use the local optimizer to "repair" the obvious mistakes made by crossover, so the intentional attempt at cooperation was in only one direction.

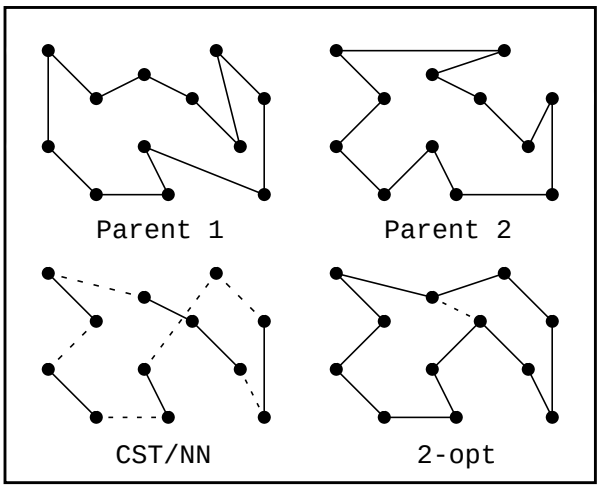


Figure 7.4: Example of CST/NN and CST/NN-2-opt. One common edge is lost (disrupted) during 2-opt.

Radcliffe's design principles (see section 2.5.1) have been expanded to include a domain-independent mutation operator--Binomial Minimal Mutation (BMM) [RS94]. Using the BMM to perform local search, a domain-independent model for hybrid operators emerges[1]. Since the Binomial Minimal Mutation for the undirected edge representation is a 2-opt swap, RRR-BMM is equivalent to a 2-opt based hybrid operator[2].

7.3.4 Results: CST/NN-2-opt vs. GX-2-opt and RRR-BMM

The CST/NN-2-opt, GX-2-opt, and RRR-BMM operators have been tested experimentally on a series of TSP instances. The initial population is seeded with 400 random 2-opt

1. Hybrid operators of this form are also called "memetic" operators.
2. The allelic hill-climber [RS94] formed from BMM for these experiments is the same as 2-opt (see section 7.1).

solutions. In these experiments, the CST/NN-2-opt solutions are better than the GX-2-opt solutions which are better than the RRR-BMM solutions. (See Table 7.1.) Further, the average time to execute 2-opt is least for restarts from CST/NN, and these times follow the same progression among the operators.

Table 7.1: Comparison of CST/NN-2-opt, GX-2-opt, and RRR-BMM on 5 TSP instances from TSPLIB. Results are for a steady-state GA with a population of 400 run until 10 generations pass without an improvement. Values are percent distance from known optimum for average of 5 runs. Average times for 2-opt are given for a SPARC 20.

TSP Instance	Avg. Best 2-opt Start	Avg. Best CST/NN-2-opt	Time (s)	Avg. Best GX-2-opt	Time (s)	Avg. Best RRR-BMM	Time (s)
d198	+ 3.06 %	+ 0.87 %	0.04	+ 1.12 %	0.06	+ 1.99 %	0.08
lin318	+ 5.16 %	+ 0.31 %	0.13	+ 0.77 %	0.21	+ 3.04 %	0.27
fl417	+ 2.54 %	+ 1.16 %	0.37	+ 1.19 %	0.51	+ 1.66 %	0.56
pcb442	+ 7.29 %	+ 1.22 %	0.36	+ 2.28 %	0.52	+ 5.61 %	0.61
u574	+ 8.26 %	+ 2.68 %	0.83	+ 3.66 %	1.00	+ 6.75 %	1.14
average	+ 5.26 %	+ 1.25 %		+ 1.80 %		+ 3.81 %	

All of the initial crossover operators are effective at preserving the common edges which define the big valley structure for the TSP. (See Table 5.1.) However, the initially preserved common edges can be disrupted during the 2-opt procedure. Despite these losses, the final CST/NN-2-opt offspring keep over 90% of the common (CST) edges from their parents. (See Table 7.2.) Conversely, 2.6% more of these common edges are disrupted in GX-2-opt, and 9.9% more are disrupted in RRR-BMM.

Table 7.2: Average percentage of common edges in the parents that are kept in the final offspring solution. To avoid convergence effects, data is only collected during the first generation.

TSP Instance	CST/NN-2-opt	GX-2-opt	RRR-BMM
d198	89.9 %	87.1 %	80.7 %
lin318	93.5 %	92.1 %	86.8 %
fl417	86.6 %	83.2 %	76.2 %
pcb442	91.1 %	87.9 %	77.8 %
u574	89.7 %	87.5 %	80.0 %
average	90.2 %	87.6 %	80.3 %

The number of disrupted common edges is a measure of the distance between the final offspring and its original parents. Since fitness information from the current parents might not apply to distant neighbors, a "GA should explore ... new regions [that] are not too far ... from the currently exploited regions" [MWS91]. Thus, a hybrid operator which disrupts fewer common edges should also find better solutions. Conversely, a hybrid operator which disrupts too many common edges is unable to benefit from the above-average fitness of its parents. (See Table 7.3.)

Table 7.3: Average improvement in fitness from the original parents to their final offspring. To allow comparisons with the edge preservation results, data is again collected from only the first generation.

TSP Instance	CST/NN-2-opt	GX-2-opt	RRR-BMM
d198	- 0.04 %	- 0.23 %	- 0.89 %
lin318	+ 0.56 %	+ 0.19 %	- 1.03 %
fl417	- 1.49 %	- 1.71 %	- 2.52 %
pcb442	+ 1.11 %	+ 1.00 %	- 0.79 %
u574	+ 0.82 %	+ 0.52 %	- 0.76 %
average	+ 0.19 %	- 0.05 %	- 1.20 %

For the TSP, the number of disrupted common edges is also an implicit measure of the distance between the initial crossover solution and the big valley of local optima. When the initial crossover solution is closer to the big valley, the inefficient process of bringing this start solution into the near optimal region is reduced. In addition to finding better solutions, the 2-opt local optimizer is also more (time) efficient when it is restarted from a CST/NN solution. (See Table 7.1.)

7.3.5 The Role of Crossover in a Hybrid Operator

It is argued that a weak, poorly matched, or otherwise poorly designed crossover operator will act as little more than a random restart method. In the previous hybrid operators, the 2-opt local optimizer repairs the mistakes of crossover. Specifically, crossover has not been *matched* to the local optimizer. The following experiment compares hybrid operators with random restart.

In random search, the best solution is found with equal probability at any time. For a series of random trials, a graph of when the best solution is found should approximate a uniform distribution. Conversely, the graph for a hybrid operator should be zero while the search process improves upon the earlier solutions. After this initial phase, the hybrid GA can either converge, or it can degrade into a random search. The graph for convergence should be a large peak, and the graph for "pseudo-random restart" should again approximate a flat line.

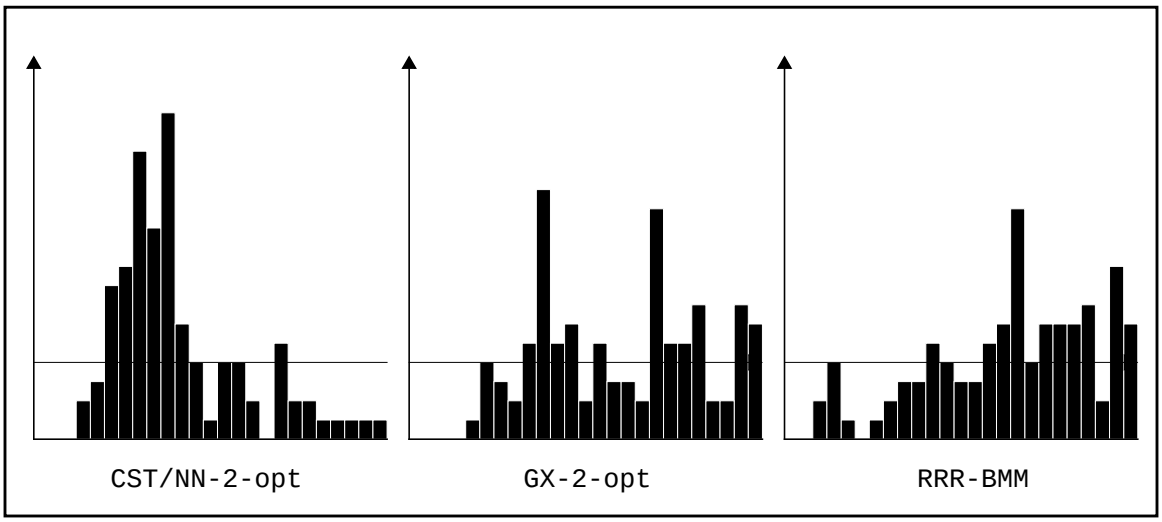


Figure 7.5: Generation with best solution in 100 independent trials. Bars represent 10 generations each. The horizontal line displays the approximate (uniform) distribution that would be expected for random restart.

This experiment has been conducted on the lin318 instance. Using a steady-state GA with an initial population of 400 random 2-opt solutions, CST/NN-2-opt, GX-2-opt, and RRR-BMM are run for 250 generations each. In 100 independent trials, the generation which contains the best solution is recorded in bar graphs. (See Figure 7.5.)

All of the bar graphs are zero for the first 20 generations. For random search, this event occurs with a 2.39×10^{-4} probability. In addition to this initial search phase, CST/NN-2-opt shows a strong convergence around 80 generations, RRR-BMM is roughly flat after 100 generations, and GX-2-opt is somewhere in between. These results confirm the ability of CST/NN-2-opt (and the inability of RRR-BMM) to conduct neighborhood search in the globally convex search space of the TSP.

7.4 Discussion

The CST/NN-2-opt commonality-based hybrid operator finds the best solutions, is the most time efficient, and has the strongest search convergence. All of these attributes are derived from CST/NN. Specifically, the higher quality start solutions reduce the work load (computational time) of the local optimizer. Since the "travel" induced by local optimization is also reduced, there is more focus (convergence) to the overall search process. This focus is desirable when good solutions clustered in a big valley.

Conversely, GX and RRR are weaker than CST/NN as independent operators, and they lead to weaker hybrid operators. The GX-2-opt and RRR-BMM hybrid operators are less efficient and less effective than CST/NN-2-opt. The distance between parent solutions and the final offspring may have exceeded the "exploratory horizon beyond which genetic search degrades to random search" [MWS91] for these operators. A hybrid GA is more likely to perform *neighborhood* search when it integrates a well-designed, well-matched crossover operator.

The Adaptive Multi-Start procedure uses the equivalent of a domain-independent crossover operator to generate its start points. Since domain-independent operators (e.g. RRR) can lead to relatively weak hybrid operators, the non-heuristically generated adaptive starting tours may be responsible for the poor overall performance of AMS. Further, the multi-parent nature of the AMS restart operator creates larger neighborhoods which can divert the focus of AMS away from the structure of the big valley. By avoiding these pitfalls, the Commonality-Based Crossover Framework provides a better design model for restart operators.

7.5 Additional Comments

The results reported for CHC [Esh91] are much better than the observed results for RRR-BMM. The base crossover operator in CHC is (effectively) RRR, but two-repair (a modified form of 2-opt that preserves all common edges) is the local optimizer. Two-repair allows better exploitation of common components, and massive mutation during (CHC) restarts allows exploration.

Exploration can also be achieved by using (single parent) “kick” operators[1]. Since the purpose of a kick operator is to escape from the neighborhood of the current local optima, hybrid operators of this form are clearly intended as best-of-k-runs approaches. As single-parent operators, these methods cannot explicitly exploit common components. However, their strong results suggest this doesn’t matter with certain local optimizers (e.g. Lin-Kernighan [LK73]).

7.6 Summary

It may be possible for hybrid operators to benefit from the new design model. Although these experiments involved a relatively weak local optimizer (i.e. 2-opt), it was observed that the fitter initial start solutions of CST/NN were able to reduce the work load of the local optimizer. Further, the preserved common components were matched to the structure of the big valley (i.e. edges for the TSP). In CST/NN-2-opt, the search process focused in the smallest neighborhood around its parent solutions, and it performed best overall. However, the effectiveness of kick operators contradicts the importance of common components in restart methods.

1. The “double bridge” (4-opt) kick operator is widely regarded as the best restart method for the TSP [Rei94][JM97].

Chapter 8

Vehicle Routing

The Commonality-Based Crossover Framework has been applied to vehicle routing problems. Common Clusters are used as the initial partial solution for two problem variations. The effectiveness of the resulting operators supports the general value of common components.

8.1 Overview

Vehicle routing problems are too complex to solve by exact methods [DDS92]. Thus, heuristic methods are the primary optimization technique. Since the solution quality for many of these methods has been reported on the available benchmark problems, vehicle routing provides an ideal problem domain to examine the practical value of the Commonality-Based Crossover Framework.

Vehicle routing problems are derived from the Traveling Salesman Problem--the "salesman" is replaced by capacity-constrained "vehicles". Further, depending on the modeled conditions, additional constraints (e.g. time windows) are often imposed. These domain specific (non-representation level) constraints compound the (representation level) constraints inherent to sequences--which best represent routes. Overall, it is difficult for (random) recombination to develop feasible offspring.

The common schemata of two feasible parents define a search space with at least two feasible solutions (i.e. the parents). Using a "cluster first, route second" strategy, the Common Clusters (which consist of customers served by the same vehicle in both parents) are preserved. This process acts like a dynamic clustering algorithm--parent fitness updates the clustering criteria. Completing this partial solution by Insertion, the Common Clusters/Insertion (CC/I) heuristic operator is developed.

The new heuristic operator has been tested on two variations of the vehicle routing problem. Experiments show that CC/I performs better than previous GA approaches, but it is not competitive with the best available methods. However, the best methods tend to be hybrid (restart) techniques. For a better comparison, CC/I has been paired with the Or-opt local optimizer [Or76]. In preliminary experiments, the Common Clusters/ Insertion-Or-opt hybrid operator has found new best-known solutions on five instances of the Vehicle Routing Problem with Time Windows.

8.2 Problem Formulations

Vehicle routing problems model the servicing of "customers" by "vehicles". Examples include picking up children by school busses, delivering parcels by couriers, and reading meters by inspectors. In general, these problems involve servicing a set of N customers

c_i from a depot c_0. Each customer has a quantity requirement q_i and a time requirement t_i, and each vehicle has a maximum capacity Q and a time limit T. Each vehicle (which must start and finish at the depot) takes time t_{ij}, equal to the (Euclidean) distance $d(c_i, c_j)$, to travel between customers. Building upon these basic features, the definitions of the (Capacitated) Vehicle Routing Problem and the Vehicle Routing Problem with Time Windows follow.

8.2.1 The (Capacitated) Vehicle Routing Problem

Since it is the base form, the Capacitated Vehicle Routing Problem is often referred to as just the Vehicle Routing Problem (VRP). The assertion of capacity constraints is redundant because the VRP reverts back to the TSP without them. The most popular benchmark problems for the VRP have been developed by Christofides [CMT79].

In the VRP, the first objective is to minimize the total number of vehicles K that are used to service the customers. The (overhead) cost of adding an extra vehicle is much larger than the incremental cost of operating an existing vehicle. Therefore, the second objective is to minimize operating costs. These costs are usually represented by the total travel distance D:

$$(8.1) \quad D = \sum_{k=1}^{K} d_k .$$

In equation (8.1), d_k represents the distance traveled by vehicle k to sequentially visit the n_k customers on its route π_k. Specifically, the distance each vehicle travels to visit its customers is represented by

$$(8.2) \quad d_k = d(c_0, c_{\pi_k(1)}) + \sum_{j=1}^{n_k - 1} d(c_{\pi_k(j)}, c_{\pi_k(j+1)}) + d(c_{\pi_k(n_k)}, c_0).$$

The customers that can be included on a route π_k are subject to the vehicle's capacity constraint,

$$(8.3) \quad Q \geq \sum_{i=1}^{N} x_{ik} \cdot q_i ,$$

and time constraint,

(8.4) $T \geq$ travel time + service time

(8.5) $$T \geq d_k + \sum_{i=1}^{N} x_{ik} \cdot t_i .$$

The Boolean variable x_{ik} in equations (8.3) and (8.5) identifies which customers are serviced by vehicle k on route π_k.

(8.6) $$x_{ik} = \begin{cases} 1 & i \in \pi_k \\ 0 & i \notin \pi_k \end{cases}$$

Naturally, all customers must be serviced once and only once.

(8.7) $$\sum_{k=1}^{K} x_{ik} = 1$$

8.2.2 The Vehicle Routing Problem with Time Windows

The basic VRP does not sufficiently model certain real world conditions. For example, children cannot be picked up before classes are over, and parcels cannot be delivered after a customer's business hours. To handle these additional constraints, the Vehicle Routing Problem with Time Windows (VRPTW) requires each customer c_i to be serviced within a time window defined by an earliest service time f_i and a latest service time l_i. If the vehicle arrives early, it must wait until f_i to begin servicing the customer. Conversely, if the vehicle arrives late, the solution is infeasible. Otherwise, the VRPTW has the same objectives and constraints as the VRP. The most popular benchmark problems for the VRPTW have been developed by Solomon [Sol87].

8.3 Previous Genetic Algorithms for Vehicle Routing

For the VRP, a Genetic Algorithm with the Petal Method [Hjo93] has been tested on the problems developed by Christofides. For the VRPTW, the GIDEON GA-based system [Tha93] has been tested on the problems developed by Solomon. Both of these GAs focus on combination.

8.3.1 A Genetic Algorithm with the Petal Method

The Genetic Algorithm with the Petal Method (GAPM) [Hjo93] uses a (blind) “seed route crossover” (which behaves like Order Crossover--see section 4.2.3) to combine parent solutions into new cyclic orders (sequences). These cyclic orders are transformed/ decoded into VRP solutions by the Petal Method. When a cyclic order is decoded, adjacency relationships (edges) are used to form petals. Thus, the building blocks manipulated by the (order-based) seed route crossover operator might not match the structure of the Petal Method.

8.3.2 GIDEON

The GIDEON system [Tha93] uses a cluster first, route second decomposition. It starts with a genetic (sectoring) algorithm to cluster customers, it follows with an insertion-based heuristic to route the customers, and it finishes with a λ-interchange local optimization process to improve the initial routes. However, GIDEON is not a hybrid operator as previously defined (see chapter 7) because the genetic algorithm runs to completion before the local optimizer is invoked. The quality of this initial solution is not reported, so it is difficult to isolate the effectiveness of the genetic algorithm. Nonetheless, geometric building blocks (from sectoring) are likely an insufficient basis to support a highly effective GA--these building blocks do not consider the time and quantity requirements of the customers.

8.4 Common Clusters/Insertion

To design a commonality-based crossover operator, it is necessary to select a basis of commonality. Since the sequencing (routing) problem for each vehicle is defined by the customers it is assigned, these assignments form the basis of commonality. Customers that are serviced by the same vehicle in both parent solutions are identified as clusters. The largest “independent” clusters (of at least 2 customers each) are preserved by Common Clusters. (See Figure 8.1.)

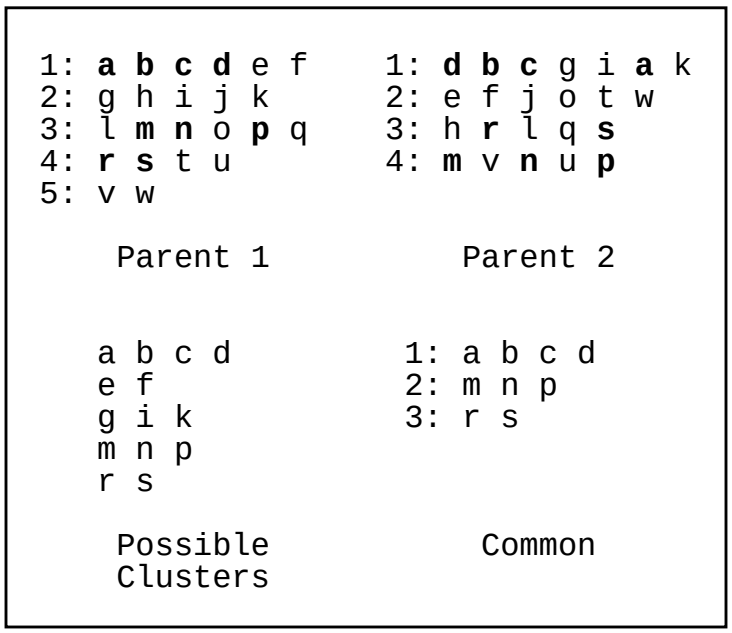


Figure 8.1: Example of Common Clusters. The largest cluster (`abcd`) is chosen first. The `ef` and `gik` clusters are not independent to it. If `gik` was also chosen, then Parent 2 could not be built by Insertion.

An initial route for each of the Common Clusters is developed by Arbitrary Insertion (see section 5.3). The order to add the remaining customers is determined by selecting three random customers, and then returning the one farthest away from the depot[1]. By favoring the early addition of distant customers, routes with only distant customers are more likely to be developed. By reducing the number of vehicles that service distant customers, the total distance `D` is often reduced. (See Figure 8.2.)

After choosing which customer will be added next, its vehicle and route location are determined by Insertion--the customer is inserted in each route location of each vehicle, and the feasible solution which incurs the least incremental cost is returned. If it is not feasible to service the customer on any of the current routes, a new vehicle is added. Overall, this process defines the Common Clusters/Insertion heuristic operator.

1. A randomized insertion order favors diversity--random errors versus systematic errors.

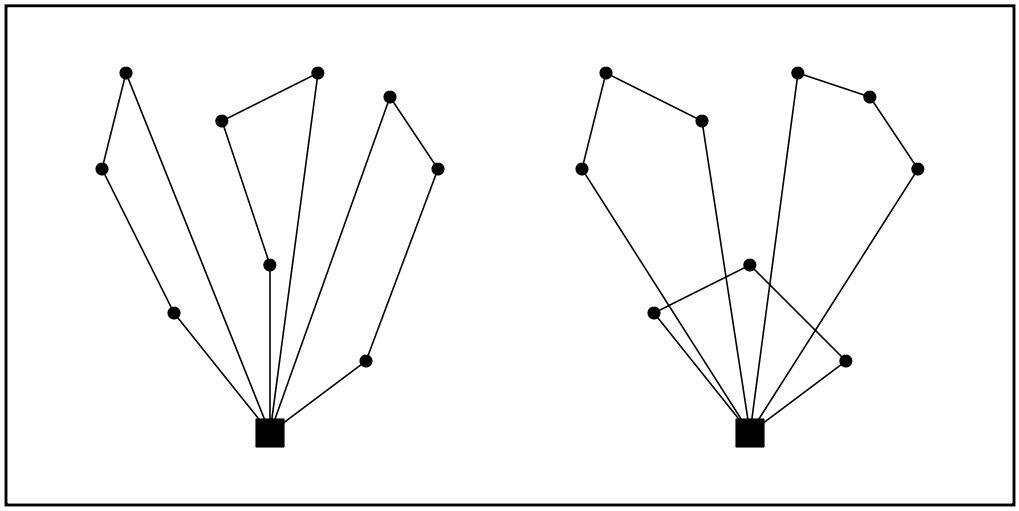


Figure 8.2: Example of VRP solutions. It is usually desirable to service the distant customers with fewer vehicles.

8.5 Results for the Vehicle Routing Problem

Common Clusters/Insertion has been tested on the Christofides VRP instances. In these experiments, the population size is set to 2N, and it is initialized with random Insertion solutions[1]. Using a steady-state GA (2-tournament parent selection, remove worst, no duplicate solutions), the stop condition is 10 generations without an improvement to the best overall solution.

The results for Common Clusters/Insertion are given as percent distance above the best-known solutions [Tai93] for the average of 5 runs. The results for GAPM appear to be for a single run. Since there are no differences in the number of vehicles K, only results for the overall distance D are shown. (See Table 8.1.) The solutions found by CC/I are better and more consistent than solutions found by GAPM.

1. Using capacity to determine the minimum number of vehicles, a random customer is assigned to each of these routes. The remaining customers are then added in 3-tournament order by Insertion (see section 8.4).

Table 8.1: Performance of CC/I and GA with the Petal Method on Christofides VRP instances. Values are percent distance above best-known solutions.

VRP Instance	Size (N)	Common Clusters/ Insertion	GA with the Petal Method
1	50	+ 0.45 %	+ 0.0 %
2	75	+ 2.27 %	+ 4.5 %
3	100	+ 1.30 %	+ 0.7 %
4	150	+ 2.57 %	+ 4.9 %
5	199	+ 2.96 %	+ 6.2 %
1 - 5		+ 1.91 %	+ 3.3 %
6	50	+ 0.13 %	
7	75	+ 1.70 %	
8	100	+ 0.64 %	
9	150	+ 3.43 %	
10	199	+ 2.75 %	
11	120	+ 3.77 %	
12	100	+ 0.13 %	
13	120	+ 2.81 %	
14	100	+ 0.42 %	
1 - 14		+ 1.81 %	

The Petal Method finds the optimal petal solution for a given cyclic order. Thus, it transforms the VRP into the problem of finding the optimal cyclic (seed) order. Essentially, the Petal Method decodes genotype solutions of cyclic orders into phenotype solutions of vehicle and route assignments. Fitness-based selection and random recombination are then used to find better cyclic orders/VRP solutions.

Unfortunately, the performance of blind operators is not domain independent (see section 4.2). The (random) schemata combined during crossover must still match the structure (building blocks) of the objective function (decoder). Otherwise, the resulting genetic algorithm may not perform much more than an elaborate random search. Since the results for GAPM are relatively poor, it appears that the (order-based) seed route crossover operator may not properly match the genotype search space defined by the (edge-based) Petal Method.

Table 8.2: Performance of CC/I and GIDEON on Solomon VRPTW instances. The better solutions appear in bold.

VRPTW Instance	GIDEON		Common Clusters/ Insertion		VRPTW Instance	GIDEON		Common Clusters/ Insertion	
	Vehicles	Distance	Vehicles	Distance		Vehicles	Distance	Vehicles	Distance
R101	20	**1700**	20	1799.41	R201	4	1478	4	**1265.79**
R102	17	**1549**	17	1639.40	R202	4	1279	4	**1111.58**
R103	**13**	**1319**	14	1280.18	R203	3	1167	3	**1065.33**
R104	10	1090	10	**1017.71**	R204	3	909	3	**768.61**
R105	15	1448	**14**	**1466.34**	R205	3	1274	3	**1247.63**
R106	13	1363	13	**1247.99**	R206	3	1098	3	**1021.10**
R107	11	1187	11	**1122.91**	R207	3	1015	3	**886.88**
R108	10	1048	10	**980.84**	R208	3	826	**2**	**815.50**
R109	12	1345	12	**1216.48**	R209	3	**1159**	3	1227.26
R110	**11**	**1234**	12	1110.19	R210	3	1269	3	**1122.89**
R111	11	1238	11	**1155.53**	R211	3	898	3	**811.35**
R112	10	**1082**	10	1180.05					
C101	10	833	10	**828.94**	C201	3	753	3	**591.56**
C102	10	832	10	**828.94**	C202	3	756	3	**591.56**
C103	10	873	10	**828.06**	C203	3	855	3	**591.17**
C104	10	904	10	**825.54**	C204	3	803	3	**596.55**
C105	10	874	10	**828.94**	C205	3	667	3	**588.88**
C106	10	902	10	**828.94**	C206	3	694	3	**588.49**
C107	10	926	10	**828.94**	C207	3	730	3	**588.29**
C108	10	928	10	**828.94**	C208	3	735	3	**588.32**
C109	10	957	10	**828.94**					
RC101	**15**	**1767**	16	1681.33	RC201	4	1823	4	**1534.95**
RC102	14	1569	14	**1507.03**	RC202	4	1459	4	**1245.29**
RC103	11	**1328**	11	1388.67	RC203	3	**1323**	3	1430.52
RC104	11	1263	**10**	**1186.92**	RC204	3	1021	3	**836.74**
RC105	**14**	**1612**	15	1590.66	RC205	4	1594	4	**1404.30**
RC106	**12**	**1608**	13	1447.99	RC206	**3**	**1530**	4	1105.78
RC107	12	1396	12	**1315.54**	RC207	**3**	**1501**	4	1034.75
RC108	11	1250	11	**1141.88**	RC208	3	1038	3	**929.67**

8.6 Results for the Vehicle Routing Problem with Time Windows

With a minor modification, Insertion can be redesigned to handle time window constraints. The resulting version of Common Clusters/Insertion has been applied to the Solomon VRPTW instances. This version of CC/I has been extended into a hybrid operator by pairing it with the Or-opt local optimizer.

8.6.1 Common Clusters/Insertion vs. GIDEON

In GIDEON, five (linked) cycles of the GA and λ-interchange local optimizer are run, and the best solution is returned. For the CC/I experiments, the same GA parameters presented in the previous section are used--steady-state replacement, population size $2N$[1], random Insertion seed solutions, and a stop condition of 10 generations without an improvement. Five independent trials are run, and the best result is reported. (See Table 8.2.) The solutions found by CC/I are generally better than those found by GIDEON[2], even though CC/I solutions are not locally optimized.

The initial quality of the GA solutions within GIDEON are not reported. This implies that the role of crossover (and the overall GA) is to provide coarse start points for the λ-interchange local optimizer. However, the fitter CC/I solutions should provide better start points for a local optimizer.

8.6.2 Common Clusters/Insertion-Or-opt

The Or-opt local optimizer uses Or-opt exchanges[3] [Or76] to perform a greedy search. Starting with a complete feasible solution, sequences of three consecutive customers are moved to other feasible locations within the same route and in other routes. Next, sequences of two consecutive customers are tried, and then single customers are tried. If an improving move is found, the procedure is restarted immediately from the new solution (i.e. random hill climbing). The procedure is repeated until a locally optimal solution is found.

---

1. N = 100 for all of Solomon's VRPTW instances.
2. Results for GIDEON are reported as integral values, not the preferred double-precision floating point.
3. Or-opt exchanges are a subset of 3-opt exchanges.

Appending the Or-opt local optimizer to CC/I, the Common Clusters/Insertion-Or-opt hybrid operator is developed. In preliminary experiments (same parameters with random Insertion-Or-opt seed solutions), the commonality-based hybrid operator finds new best-known solutions to five VRPTW instances. (See Table 8.3.) Unfortunately, the time performance of CC/I-Or-opt is significantly worse than the previous methods. Rather than claim that the new hybrid operator is competitive with these methods, it is claimed that CC/I shows promise as a restart method. In particular, Or-opt is much weaker than the tabu search procedures used by the best VRPTW methods [Tai93][TBG97].

Table 8.3: New best-known VRPTW solutions found by CC/I-Or-opt.

VRPTW Instance	Common Clusters/Insertion-Or-opt		Previous Best		
	Vehicles	Distance	Vehicles	Distance	Reference
R201	4	1253.23	4	1254.80	[TBG97]
R210	3	961.59	3	967.50	[RT95]
RC204	3	798.73	3	806.75	[RT95]
RC205	4	1309.73	4	1328.21	[TBG97]
RC208	3	832.36	3	833.97	[RT95]

8.7 Discussion

Due to the complex constraints of vehicle routing problems, (random) recombination rarely produces feasible offspring. The required repair operations and/or decoders can complicate the identification of building blocks. In particular, certain decoders (e.g. dispatch rules) cause good solutions to become randomly distributed in the (genotype) search space [MBK97]. Under these conditions, one good solution cannot be used to help find other good solutions. Subsequently, neighborhood search is not possible. This design flaw may have occurred in GAPM and GIDEON--although they incorporate strong local search techniques, they still perform poorly.

Unlike combination, it is relatively easy to design a commonality-based crossover operator that will maintain constraints. Specifically, the schemata common to two feasible parents define a search space with at least two feasible solutions (i.e. the parents). If the remaining constraints can be satisfied by the construction heuristic[1], the overall

search process will stay within the feasible region. This allows decoders and repair operations to be avoided.

As part of a cluster first, route second procedure, geometric (distance) information is often used to create clusters [Tai93][Tha93]. However, distance is not the only factor that determines the compatibility of customers (e.g. time windows and capacity requirements). Common Clusters (implicitly) considers all possible factors when it accumulates information on previous above-average (locally optimized) routes. This information allows Common Clusters/Insertion to develop new start solutions that are closer to the (locally optimal) parent solutions. These start solutions should improve the efficiency and effectiveness of the local optimizers (see section 7.3).

8.8 Summary

The Common Clusters/Insertion heuristic operator is more effective than GAPM and GIDEON. Since these experiments involve two variations (the VRP and the VRPTW), they substantiate the general value of common components. An attempt to extend this value to a novel hybrid operator for the VRPTW is suggested below. The preliminary work to this extension has already discovered new best-known solutions to five instances.

8.9 Extension

The previous experiments used a simple Insertion heuristic, and the Or-opt local optimizer is weaker than recently developed tabu search procedures. To improve performance, Common Clusters can restart any of Solomon's insertion variations [Sol87], and any (or all) of these "new" heuristic operators can be paired with the various local optimizers that are available. However, these extensions still handle both objectives (minimizing vehicles and distance) simultaneously. Conversely, a hybrid operator can pair together two quite different operators (e.g. operators with different objectives). Specialization could allow the heuristic operator to focus on one objective, and the local optimizer to focus on the other.

1. It is assumed that feasible solutions are relatively easy to find--that the primary challenge is optimization. If feasible solutions are relatively scarce, constraint satisfaction techniques (to find feasible solutions) may be more appropriate.

In the VRPTW experiments with CC/I-Or-opt, vehicle reductions appear difficult to achieve during the local optimization stage. Since local optimizers seem better suited to address the distance objective, the heuristic operator should focus strictly on the vehicles objective. Unfortunately, the distance-based insertion heuristics used by GIDEON, Common Clusters/Insertion, and the tabu search hybrid system of Taillard et al [TBG97] have not been designed to optimize a "vehicles-only" objective.

The elimination of distance from the (insertion) objective should make it easier to construct solutions that use the minimum number of vehicles. Although construction heuristics that focus strictly on minimizing vehicles do not seem to exist, they should be relatively easy to develop from operating system principles. Specifically, packing the time windows of customers onto routes is similar to the allocation of core memory to CPU processes. As it is desirable to place processes in memory such that the remaining "holes" are still useful [SPG91], it is equally desirable to assign customers to vehicles such that the remaining idle times can be productively filled.

With the proper basis of commonality, the above "packing" heuristic can be extended into a heuristic operator. Since the Common Clusters implicitly consider many aspects (e.g. capacity and time windows) when determining the compatibility of customers, it should still identify useful building blocks for a vehicles-only objective. With the implicit consideration of distance, Common Clusters also prepares the resulting "Common Clusters/Packing" heuristic operator to be paired with a distance-based local optimizer.

Or-opt is expected to be ineffective as the distance-based local optimizer. When the initial routes are tightly packed, there is not enough space to accept additional customers during Or-opt exchanges. Thus, λ-interchanges (which can swap customers between routes) may be required. Since most tabu search procedures are based on λ-interchanges, they should be quite effective in post-processing Common Clusters/Packing solutions--especially if they focus on distance only.

Chapter 9

Search Space Reductions (with Applications to Flow Shop Scheduling)

Commonality-based crossover operators will preserve matched constraints at the representation level. These constraints can be used to (transparently) reduce the search space. When applied to flow shop scheduling problems with order-based objectives, Precedence Preservative Crossover with Edges performs better than Uniform Order-Based Crossover--the previous best sequencing operator for order-based objectives.

9.1 Overview

Maximum Partial Order/Arbitrary Insertion performs better (in relative terms) on the Sequential Ordering Problem than on the Traveling Salesman Problem (see section 5.3). The precedence constraints in the SOP seem to help the (order-based) MPO/AI operator--more constraints increase the relative performance. This observation suggests that certain constraints can be beneficial to commonality-based operators. These constraints cause (transparent) *search space reductions*[1]--the preservation of common components will also preserve the satisfied constraints.

When constraints are added heuristically, the optimal solution may be eliminated from the search space. However, these reductions may still allow a better solution to be found during a time-limited search. For example, it is a standard textbook proposition that the sampling of non-delay schedules will be more productive than the sampling of active schedules--even though the optimal schedule may be active, but not non-delay [CMM67][Fre82]. In general, problem domains which require computational efficiency should benefit more from a reduced search space.

Search space reductions have been applied to flow shop scheduling problems. When single-queue factories (a superset of flow shops) with order-based cost objectives (e.g. tardiness and earliness) are modeled by simulation, genetic algorithms are the best optimization technique [RHW96][WHR98]. With search space reductions, the performance of blind sequencing operators (and commonality-based operators in particular) improves further.

9.2 Flow Shop Scheduling

When the factory is modeled by simulation, the “black box” could (interchangeably) represent a single machine, a flow shop, or a single-queue factory. For computational simplicity, a two-machine flow shop is used in these experiments. However, since these problems include sequence dependent set-up times, they are still NP-complete. The choice of this object (hidden in the black box) has little influence on GA design. Conversely, the basis of the objectives is critically important--order-based cost penalties

1. Search space reductions have also been developed at the phenotype level [Mat99].

require order-based sequencing operators, and order-based constraints should be used to reduce the search space.

9.2.1 Random Flow Shop Problems

A series of random two-machine flow shop problems has been generated. For these problems, 500 independent jobs must be processed in the same sequence on both machines. The jobs have a processing time on each machine, a sequence-dependent set-up time (based on their immediate predecessor), a transfer time between machines, a due date, a tardiness cost weight, and an earliness cost weight. The objective is to minimize the sum of earliness and tardiness costs.

The job parameters are drawn from uniform distributions. The ranges are 25-100 (time units) for processing times, 5-70 for set-up times, and 5-50 for transfer times. The tardiness weights have a range of 2-20, and the earliness weights have a range of 1-5. The due dates are uniformly distributed from time 0 to the average expected makespan (50,000).

Five problem instances have been generated. Each instance consists of six 500-element vectors and a 500×500 full matrix for set-up times. To evaluate a sequence, a non-delay schedule is simulated through the two-machine factory. In this simulation, the first job has no set-up time (i.e. it starts at time 0). Then, tardiness and earliness costs are calculated using the completion time of each job on machine 2.

By design, the flow shop model is easy to simulate (two machines) but difficult to analyze. In particular, the sequence dependent set-up times should cause local search operations (e.g. swapping two jobs) to have non-localized effects (i.e. chaos--small changes have large effects). Since these chaotic interactions are an important feature of real-world factories, the intended complexity of the model allows the results to represent general environments (e.g. larger flow shops and single queue factories).

9.2.2 A Building Block Analysis

Fitness-based selection is only useful when crossover manipulates the correct building blocks (see section 4.2). In most scheduling problems, the objectives are based on two relationships: job adjacency (if job `i` *immediately* precedes job `j`, then job `i` and job `j`

are adjacent) and job order. For example, the makespan objective requires (sequence-dependent) set-up times to be minimized. Since a job's set-up time depends primarily on its immediate predecessor, makespan is an adjacency-based objective. Conversely, tardiness and earliness are order-based objectives--the cost of a job depends more on its approximate order than on its immediate neighbors.

In the developed flow shop problems, the objective is to minimize tardiness and earliness. Therefore, crossover should manipulate order-based schemata, and search space reductions should be implemented with order-based (precedence) constraints. For a precedence constraint which requires job `i` to be processed before job `j`, two feasible parents will both process job `i` before job `j`. Subsequently, a commonality-based operator can maintain this constraint transparently--as a common order-based schema, it is preserved.

9.3 Sequence-Based Operators (for Flow Shop Scheduling)

The previously presented sequence-based operators (see section 4.2) perform poorly on flow shop scheduling problems. Due to the order-based objectives, operators which manipulate position-based and edge-based schemata are inappropriate (e.g. PMX, CX, and ER). Further, the order-based operators are also ineffective--OX "wraps around", and Matrix Intersection has an $O(n^2)$ time complexity. Overall, it has been suggested that Uniform Order-Based Crossover (UX) [Sys91] is the best operator for order-based scheduling problems [SWM92].

Uniform Order-Based Crossover combines random (order-based) schemata taken from the parents, but it does not guarantee that the schemata common to both parents are preserved. Thus, UX can produce an "infeasible" offspring from two feasible parents. Conversely, Precedence Preservative Crossover (PPX) [BMK96] is an order-based operator that maintains all common precedence relationships. For unconstrained search, PPX is less effective than UX. However, by preserving the added precedence constraints, PPX should explore a reduced search space better than UX. The UX and PPX operators are hereby reviewed to highlight their effects on (common) order/precedence schemata.

9.3.1 Uniform Order-Based Crossover

Acting directly on permutation sequences, Uniform Order-Based Crossover uses a uniform crossover mask to select jobs. When the mask has a `1`, it takes the job of Parent 1 and places it in the offspring at the same site. The remaining jobs are filled into the empty sites in the order they appear in Parent 2. (See Figure 9.1.) Overall, UX combines order (and position) information from Parent 1 with order information from Parent 2. However, if a (common) order relationship is not taken from a single parent, it can be reversed.

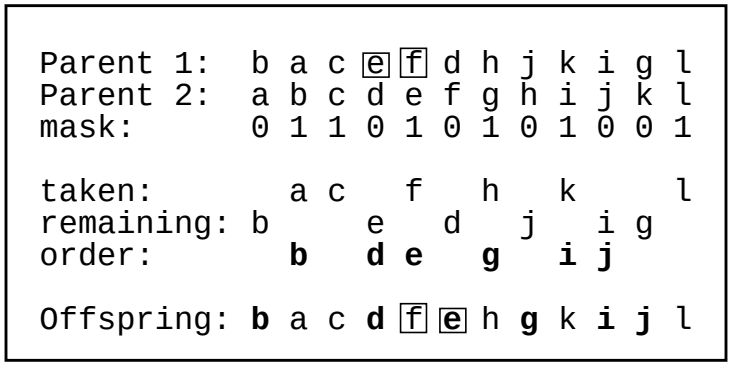


Figure 9.1: Example of UX. Common order for jobs `e` and `f` is not transferred by a single parent. Therefore, their order can be reversed in the offspring.

9.3.2 Precedence Preservative Crossover

On a sequence representation, Precedence Preservative Crossover uses a uniform crossover mask to select the parent from which to *draw* the next job. The selected parent is scanned for the first undrawn job, and this job is appended to the offspring. (See Figure 9.2.) This process of "drawing" the jobs guarantees that all common precedence relations are preserved. Subsequently, PPX will also enforce precedence constraints transparently.

Arguably, PPX is just a natural representation form of Matrix Intersection. Both operators preserve all of the common precedence relationships that are in the parents--PPX implicitly during its drawing process and MI explicitly through its Boolean matrix representation. Further, both operators fill in the remaining precedence relationships (schemata) randomly. However, by working directly on the permutation sequence representation, PPX has an $O(n)$ time complexity versus the $O(n^2)$ time complexity of MI.

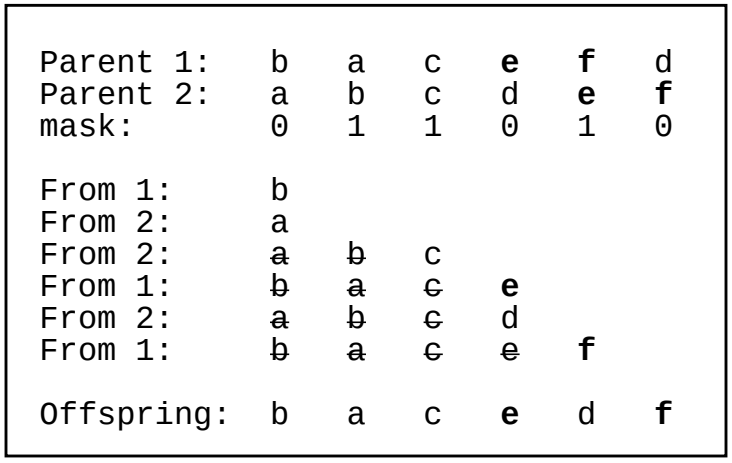


Figure 9.2: Example of PPX. Job `e` will always be drawn before job `f`.

9.4 Results for Unconstrained Search

The UX and PPX operators have been implemented in GENITOR [WS90]. The parameters are 1000 for the population size, 200,000 for the number of trials, and 2.00 for the selection bias (2-tournament selection). The results for ten runs on each of the five flow shop problems are normalized against the cost of the Earliest Due Date (EDD) dispatch sequence[1]. (See Table 9.1)

Table 9.1: Average performance of UX and PPX relative to EDD on random two-machine flow shop problems.

Instance	UX	PPX
1	0.745	7.306
2	1.409	16.550
3	1.106	14.088
4	1.490	22.071
5	0.567	5.538
average	1.063	13.111

1. EDD is used because it is independent of the factory. Most of the more advanced dispatch rules (e.g. ATC [VM87]) assume deterministic job processing times (i.e. they ignore factory dependent set-up times).

With the allowed computational effort, neither UX nor PPX performs better than EDD. The randomly initialized genetic search does not perform significantly better than a simple dispatch technique. These results support the general argument that genetic algorithms require problem specific heuristics to be competitive with the best available methods [GGR85][SG87][Dav91].

Between UX and PPX, the results with PPX are about 10 times worse. Although the commonality hypothesis suggests that schemata common to above-average solutions are above average, the components that are common to the random solutions of the initial population are likely to be equally random (i.e. not significantly above average). By over-exploiting these early building blocks, it appears that PPX converges (prematurely) in a poor region of the search space.

9.5 Search Space Reductions

To develop beneficial constraints, a promising neighborhood structure (i.e. building blocks) must be identified. Using the TSP as an example, a standard heuristic is to build tours with only the ten shortest edges of each city. A random solution in this reduced search space is much better than a completely random solution, and most of the edges in the optimal tour are still available [Rei94].

For flow shop scheduling, earliness and tardiness penalties cause jobs to have “V-shaped” cost functions. Since each job should be processed close to its EDD order, precedence constraints can be used to restrict jobs to this neighborhood. For example, if job `i` is due `x` time units after job `j`, constrain job `i` to be processed before job `j`. A series of these precedence constraints will reduce the search space, and the size of the allowed neighborhood is defined by `x`.

Precedence constraints have been developed with `x` equal to 1, 100, 300, 500, 1000, 3000, and 5000 time units. The resulting constraints define neighborhoods with an average of 0, 2, 6, 10, 20, 60, and 100 non-EDD positions for each job. Since due dates are an average of 100 time units apart, one additional position (on each side) can be expected for each such increase in `x`.

9.6 Results with Search Space Reductions

The search space reductions are only enforced for the initial population (of random solutions). After this initialization, any offspring solution is allowed in the population. Using the same GA parameters (i.e. GENITOR, 200,000 solutions, ten runs on each instance, etc), the average performance of UX and PPX has been measured for all values of x. (See Figure 9.3.)

When x is greater than or equal to 300 time units, the results with PPX are about 40% better than UX. Overall, the cost objective is reduced by over 80% relative to the EDD sequence and to the performance of unconstrained genetic search[1]. The added precedence constraints have defined a reduced search space which contains only the most promising solutions. Since PPX samples this space aggressively, it finds better solutions than UX in the allotted time. Conversely, UX wanders out of the reduced search space and wastes time sampling less promising regions of the (overall) search space.

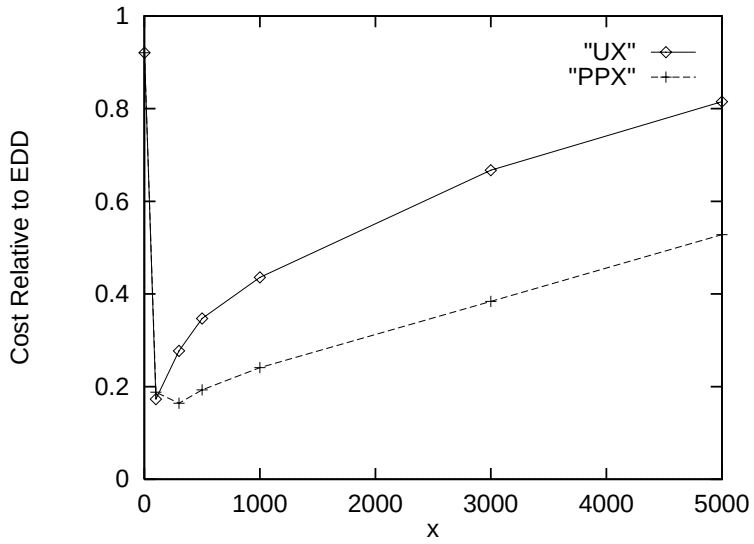


Figure 9.3: Average performance of UX and PPX for different values of x.

The unconstrained "wandering" of UX causes it to converge slower than PPX. Although this can be advantageous when the added precedence constraints are too restrictive (e.g.

1. Without bottlenecks, these problems can have very low cost solutions. For problems where the optimal solution still has a high cost, percentage cost reductions should be measured with respect to the surplus from (the unknown) optimum.

when x is 100), UX still lags PPX. (See Figure 9.4.) For larger values of x, UX probably lags PPX by an even greater amount. Thus, depending on the time limit, the performance difference between PPX and UX may increase or decrease. However, UX should always catch PPX if it is given enough time.

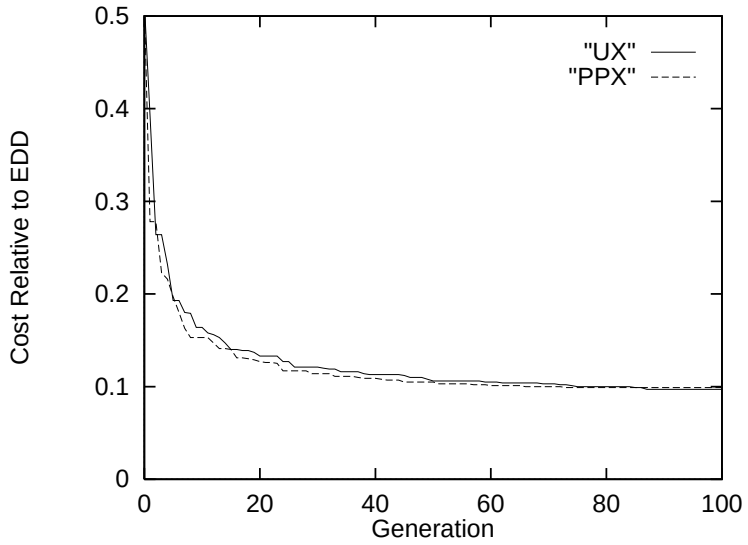


Figure 9.4: Sample run of UX and PPX on instance 1 with x equals 100.

9.7 The Role of Adjacency

Factory scheduling problems can have both adjacency-based and order-based objectives. In particular, minimizing makespan (maximizing throughput) is often an explicit objective. Regardless, it is almost always an implicit objective--it directly affects the completion time of the last job. Therefore, lowering the makespan should improve the tardiness objective.

Since the (overall) objective can be affected by both order and adjacency relationships, crossover operators should intentionally manipulate both edge-based and order-based schemata. Following this suggestion, a new sequencing operator has been developed--Precedence Preservative Crossover with Edges. This operator adds a local (edge-based) perspective to the existing global (order-based) perspective of PPX.

9.7.1 Precedence Preservative Crossover with Edges

Precedence Preservative Crossover can be trivially modified to preserve the common (directed) edges of the parents. First, scan the parents for common directed edges. Then, during the normal PPX procedure, each time the first job of a directed edge is drawn, the second job is also drawn. (See Figure 9.5.) This additional procedure transforms PPX into Precedence Preservative Crossover with Edges (PPXE).

Parent 1:	b	a	c	**e**	**f**	d
Parent 2:	a	b	c	d	**e**	**f**
mask:	0	1	1	0	1	0
From 1:	b					
From 2:	a					
From 2:	~~a~~	~~b~~	c			
From 1:	~~b~~	~~a~~	~~c~~	**ef**		
From 2:	~~a~~	~~b~~	~~c~~	d		
Offspring:	b	a	c	**e**	**f**	d

Figure 9.5: Example of PPXE. The common directed edge `e-f` is treated like a single element.

9.7.2 Results for PPXE

The performance of PPXE has been measured for all values of `x`. (See Figure 9.6.) Compared to PPX, the results for PPXE are consistently better. In addition to addressing the (implicit) adjacency-based factor within the objective, PPXE will also preserve long common "sub-tours" (e.g. `wxyz`)--a specialized order-based relationship. With search space reductions, the commonality-based Precedence Preservative Crossover with Edges operator is the best sequencing operator.

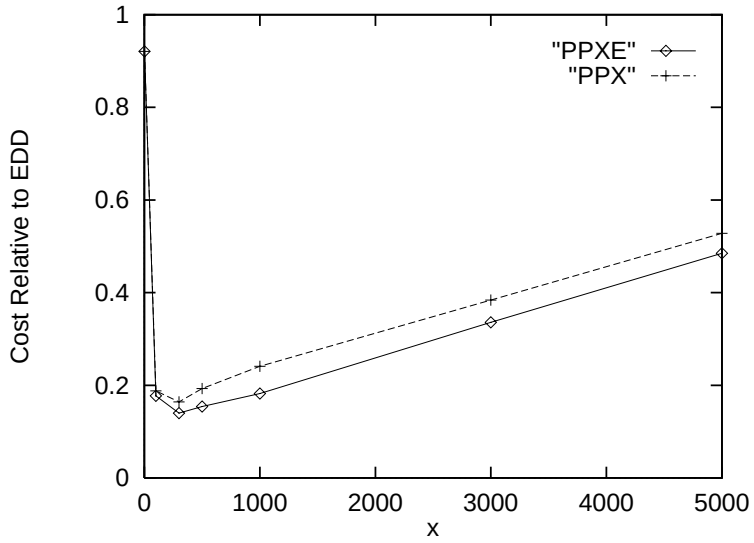


Figure 9.6: Average performance of PPXE and PPX for different values of x.

9.8 Discussion

Search space reductions can improve the performance of sequencing operators. Since these operators have not been changed, heuristic information is incorporated through the constraints. Specifically, the order-based constraints help the order-based operators find the best building blocks for the order-based objectives. The matched entities cooperate to identify and explore the most promising search space.

To benefit from heuristic constraints, they should be preserved. For constraints at the representation level[1], commonality-based operators can preserve the (satisfied) constraints of two feasible parents. Thus, the preservation of common schemata allows constraints to be handled and problem specific knowledge to be incorporated--two recurring challenges of real-world problems. Further, these constraints can be individually tailored to each problem instance and/or dynamically updated at run time (see section 13.1).

1. Certain constraints require the solution representation to be processed. For example, the time window constraints of the VRPTW (see section 8.2.2) cannot be observed in the representation alone.

9.9 Summary

Heuristic constraints have been developed for flow shop problems with order-based objectives. Operators which preserve these constraints benefit more than operators which do not. With search space reductions, Precedence Preservative Crossover with Edges performs better than Uniform Order-Based Crossover--the previous best genetic sequencing operator for black box factories with order-based objectives.

Chapter 10

A Standard Representation Problem: Feature Subset Selection

The Commonality-Based Crossover Framework has been applied to feature subset selection. Despite the standard representation, an explicit building block analysis is still necessary. Using the commonality hypothesis, a new analysis suggests that only (common) selected features are critical building blocks. By focusing on these components, the Common Features/Random Sample Climbing heuristic operator performs better than standard crossover operators.

10.1 Overview

Standard crossover operators always preserve common schemata. Thus, the first step of the new design model appears to be satisfied by default. However, the commonality hypothesis provides a new perspective for the analysis of building blocks. Through an explicit examination, the quality of the common schemata can be differentiated. By focusing on the *superior* common schemata, heuristic operators can perform better than standard crossover operators.

Feature subset selection is naturally represented by binary strings. In a solution, `1`'s cause features to be used in training (i.e. identify them as relevant), and `0`'s cause features to be ignored (as irrelevant). This standard representation "eliminates the need for designing new genetic operators" [VdJ93]. However, the counter argument is more compelling--it is "essential ... to incorporate ... local improvement operators" [SG87] to make genetic algorithms competitive with the best available methods.

A local improvement operator requires the correct building blocks (neighborhood structure) to be isolated. For feature subset selection, the critical building blocks are the "relevant" features. The commonality hypothesis, suggests that features selected in two above-average (parent) solutions (i.e. the common `1`'s) should be relevant. Conversely, it also suggests that common `0`'s (unselected features) are irrelevant. However, this (previously implicit) hypothesis is inaccurate--these features could also be weakly relevant. Due to their equal treatment of `1`'s and `0`'s, standard crossover operators are poorly suited to this standard representation problem.

A heuristic operator has been developed for feature subset selection. Since selected features (`1`'s) are the critical building blocks, the Common Features (CF) of two parents should be preserved. To complete this partial solution, Random Sample Climbing (RSC), a "constructive" local improvement operator based on $\mu+\lambda$ evolution strategies (ES), has been developed. Overall, this process defines the Common Features/Random Sample Climbing (CF/RSC) heuristic operator.

Experiments have been conducted on the RSC local improvement operator, the CF/RSC heuristic operator, a standard crossover operator, and traditional feature selection techniques. On average, the CF/RSC solutions have the smallest feature subsets, and

these subsets lead to the fewest testing errors. The larger subsets may cause the classifier to over-fit the training data. Further, it appears that (adaptive) commonality-based restarts can improve the effectiveness of ES-based methods.

10.2 Feature Subset Selection

A classification system predicts the decision class of an object based on its features. In these experiments, Euclidean Decision Tables (EDT) [GW98] are used as the classifier[1]. The feature subset selection (optimization) problem is then isolated by using the "wrapper" approach [Koh95]. When "wrapped" into the search procedure as the objective function, an EDT classifier is trained and evaluated for each candidate feature subset.

In classifier training, the features *relevant* to prediction accuracy should be used, and the *irrelevant* features should be ignored [Koh95]. This increases the "signal-to-noise ratio" of the data and decreases the training time for the classifier. Implicitly, the objective is to find the (most) relevant features. However, the explicit fitness function is to minimize the classification errors during training (with ties broken in favor of smaller subsets). This objective is used to achieve the overall goal: find the feature subset that minimizes the number of classification errors during *final testing*[2].

As a method to build classification systems, the merit of the wrapper approach has been demonstrated using basic search methods like bit climbing [Koh95]. However, most of the data sets in the original study had small feature spaces (less than 30). Since the effectiveness of search strategies is more apparent on large problems, the LandSat data set (36 features), DNA data set (180 features), and Cloud data set (204 features) are used in these experiments.

1. Results for other classifiers (including C4.5) appear in [Gue99].
2. The "best" feature subset during training can over-fit the initial training data. Thus, it may not be the best during final testing.

10.2.1 The Data Sets

A data set is a series of vectors which list all of the feature values and the assigned class for an instance. (See Figure 10.1.) The LandSat data set has 4435 training instances and 2000 testing instances of integer data representing 6 different classes. The DNA data set has 2000 training instances and 1186 testing instances of binary data representing 3 different classes. Lastly, the Cloud data set has 1633 total instances of real-value data representing 10 different classes, but no preset definition of training and testing instances has been made[1].

Instance	Feature					Class
	1	2	3	...	36	
1	92	115	120		87	3
2	84	102	106		79	3
3	84	102	102		79	3
⋮						
4435	71	91	100		81	4

Figure 10.1: Fragment of LandSat training data set.

10.2.2 Training and Testing

For the LandSat and DNA data sets, candidate feature subsets (during search) have classifiers trained on 400 instances and evaluated on 700 instances (both drawn without replacement from the training instances). The best feature subset (with the fewest training errors) is then re-evaluated with a final classifier that is trained on all of the training instances and tested on all of the testing instances. For the Cloud data set, classifiers are trained on 400 instances and evaluated on 500 instances, both drawn without replacement. Then, the final subset undergoes final testing through 10-fold cross validation. For each "fold", 60% of the data set is used for classifier training, and 40% is used for testing. The average testing errors for 10 random folds are reported.

1. The LandSat and DNA data sets are publicly available from http://www.ncc.up.pt/liacc/ML/statlog/datasets.html. The Cloud data set was provided by Richard Bankert of the Naval Research Center at Monterey, CA [Ban94].

10.2.3 A Building Block Analysis

The offspring of standard crossover operators inherit all of the common `1`'s and all of the common `0`'s from their parents. Applying the commonality hypothesis, the common `1`'s should identify relevant features and the common `0`'s should identify irrelevant features. However, the common `0`'s could also be "weakly relevant" features. The only true building blocks in feature subset selection are the selected features.

Since (common) unselected features can still be weakly relevant, they should not be eliminated from consideration. Therefore, standard crossover, as described by Convergence Controlled Variation--"allele values that are not present in the two parents cannot be introduced into the offspring" [EMS96], may be poorly suited for this (standard representation) problem. Like sequence-based operators (see section 4.2), blind operators are not necessarily domain independent--building blocks must still be analyzed.

10.3 A New Local Search Operator for Feature Subset Selection

To determine which weakly relevant features are desirable, "One possibility is to estimate which features are strongly relevant, and start the search from this subset ..." [Koh95]. Using the commonality hypothesis to identify the strongly relevant features, search should be (re)started from the common `1`'s. It has been suggested that bit climbing should perform this search [Koh95].

Bit climbing is a form of hill climbing, and probabilistic search methods (e.g. simulated annealing and tabu search) often perform better than hill climbing. Further, the Lin-Kernighan (variable-depth) heuristic [LK73] is like a $\mu+\lambda$ evolution strategies approach with μ equal to one. Combining these observations, the Random Sample Climbing local search operator has been developed for feature subset selection.

As an independent operator, Random Sample Climbing (RSC) is initialized with a seed solution of all `0`'s--no features selected. From the seed solution, λ new solutions are created by mutating up to `n` bits (these "samples" are selected randomly with replacement). If the best offspring solution is better than the previous seed solution, it becomes the new seed solution for the next generation[1] (i.e. $\mu = 1$). Overall, `k` generations of λ solutions each are generated.

Table 10.1: Results for RSC on LandSat, DNA, and Cloud data sets. Best, worst, and average values are for 30 independent trials. The best balance of breadth and depth occurs with 10 runs of 50 generations.

			Train				Test		
Data Set	Runs	k	errors			avg. subset size	errors		
			best	worst	avg.		best	worst	avg.
LandSat	1	500	52	95	78.1	14.8	220	289	242.4
	10	50	50	91	75.0	14.2	217	267	**242.2**
	25	20	55	86	75.6	13.5	216	289	246.7
	50	10	55	95	77.2	12.9	223	270	246.7
DNA	1	500	47	114	80.8	18.1	80	203	158.4
	10	50	60	87	73.0	12.0	80	174	**134.2**
	25	20	62	93	78.0	11.4	84	168	138.8
	50	10	73	100	83.5	10.1	111	167	140.5
Cloud	1	500	95	134	110.5	15.6	121.4	170.6	145.4
	10	50	82	119	102.7	19.3	114.1	159.8	132.9
	25	20	88	160	109.8	24.8	92.0	168.6	**126.7**
	50	10	93	125	108.2	18.1	117.3	158.6	133.0

When RSC starts with only a few (or even zero) selected features, mutations tend to increase the number of features[1]. Thus, RSC acts like both a construction heuristic and a local search operator. From the perspective of construction, mutations allow backtracking--features can be de-selected[2]. From the perspective of local search, multiple mutations allow escapes from one-bit neighborhood local optima. Lastly, populations ($\lambda > 1$) help reduce the negative effects of a greedy/myopic search process.

10.4 Results for Random Sample Climbing

In experiments with the RSC local search operator, n is set to 3, λ is set to 30, and 15,000 total evaluations (trained classifiers) are allowed. The available evaluations have been

1. The initial seed solution (all `0`'s) is not evaluated. It is always replaced by the best solution of the first generation.

1. RSC does not easily climb to solutions which have more than half of the available features selected.

2. Common features can also be de-selected.

distributed into one run of (k equals) 500 generations, 10 runs of 50 generations, 25 runs of 20 generations, and 50 runs of 10 generations. These parameters have each been tested on 30 different pairs of training and evaluation sets. (See Table 10.1.)

The range of results for RSC are highest when only one run of 500 generations is used. In a single run, RSC can act like a depth-first search. By analogy, more runs of fewer generations exchange breadth for depth. It appears that more breadth (runs) improve the worst trial, but that a lack of depth (generations) will negatively affect the best trial. Overall, the best balance between breadth and depth occurs with 10 runs of 50 generations each.

10.5 A Heuristic Operator for Feature Subset Selection

As a construction heuristic, the effectiveness of Random Sample Climbing should be amplified by commonality-based selection (see section 6.3). To transform RSC into a commonality-based heuristic operator, it is restarted from the Common Features (selected 1's) of two parents. The overall process defines Common Features/Random Sample Climbing (CF/RSC)--a heuristic operator for feature subset selection[1].

10.6 Results for Common Features/Random Sample Climbing

To allow direct comparisons, the experiments with CF/RSC treat n, λ, and the total number of evaluations as control variables (set to 3, 30, and 15,000 respectively). Between RSC and CF/RSC, the first uses random restarts and the second uses commonality-based restarts. The number of restarts is parameterized by k: it distributes the 500 available generations.

The value of k has been set to 20, 10, and 5, so the corresponding GAs are allowed to generate 25, 50, and 100 total solutions each. Using population sizes of 4, 7, and 10, the initial populations are seeded with RSC, and the remaining solutions are allocated to CF/RSC. These GAs are implemented in GENITOR [WS90]--1.00 is used for the selection bias (random parent selection), and duplicate solutions are disallowed.

1. The Common Features partial solution is not evaluated. This avoids the cost of an evaluation, and it forces RSC to take an initial step of exploration.

Compared to RSC alone, the results with CF/RSC are better overall. (See Table 10.2.) They also appear to be more robust across parameter settings--the average training errors have a maximum range of 3.4 (Cloud data set) for CF/RSC versus 10.5 (DNA data set) for RSC. Commonality-based restarts of the ES-based RSC seem to benefit from both breadth and depth, without sacrificing either. Overall, the best parameter set is (5, 10-90)--it finds the smallest subsets, and it has the fewest "best test errors".

Table 10.2: Results for CF/RSC on LandSat, DNA, and Cloud data sets. Best, worst, and average values are for 30 independent trials. Performance is robust across parameter settings, but (5, 10-90) leads to smaller subsets and fewer "best test errors".

				Train				Test		
Data Set	k	RSC	CF/ RSC	errors			avg. subset size	errors		
				best	worst	avg.		best	worst	avg.
LandSat	20	4	21	52	92	73.9	13.6	215	315	247.1
	10	7	43	53	90	73.8	13.4	215	275	245.2
	5	10	90	54	93	75.1	**12.8**	**205**	313	247.7
DNA	20	4	21	45	69	54.9	9.5	74	140	98.9
	10	7	43	46	68	55.8	9.3	74	126	99.3
	5	10	90	45	72	57.4	**8.5**	74	142	104.1
Cloud	20	4	21	85	115	99.7	18.4	116.2	143.3	130.6
	10	7	43	86	118	99.3	18.2	113.5	151.2	128.4
	5	10	90	90	119	102.7	**14.0**	**101.9**	141.0	124.7

10.7 Standard Crossover Operators

For standard crossover operators, Guerra-Salcedo & Whitely [GW98] have shown that CHC [Esh91] performs better than GENESIS [Gre84]. Comparing CF/RSC to CHC, the new heuristic operator performs better--even though CHC also incorporates aspects of local search (e.g. cataclysmic mutation). The constructive nature of CF/RSC and the explicit identification of strongly relevant features provide advantages over CHC and standard operators.

Table 10.3: Results for CF/RSC (5, 10-90) and CHC on LandSat, DNA, and Cloud data sets. Best, average, and standard deviation values are for 30 independent trials.

		Train				Test		
Data Set	Algorithm	accuracy (% correct)			avg. subset size	accuracy (% correct)		
		best	avg.	std. dev.		best	avg.	std. dev.
LandSat	CF/RSC	**92.3**	**89.3**	1.08	12.8	**89.8**	87.6	1.01
	CHC	86.8	85.3	0.81	12.6	88.9	87.6	1.25
DNA	CF/RSC	93.6	91.8	0.89	8.5	**93.8**	**91.2**	1.33
	CHC	**96.4**	**95.1**	0.51	11.2	92.5	89.4	2.13
Cloud	CF/RSC	82.0	79.5	1.68	14.0	**84.4**	**80.9**	1.67
	CHC	**84.8**	**82.2**	1.37	42.1	80.8	79.3	1.95

10.7.1 CHC

In the CHC algorithm, each pair of mating parents must be different by a minimum (threshold) number of bits. Essentially, CHC attempts to exploit the differences of population members, not their similarities. When there are not enough differences to exploit (i.e. the population has converged), CHC reintroduces variety by cataclysmic mutation. This form of local search reseeds the population with heavily mutated "clones" (neighbors) of the best solution.

Since CHC starts with a random population (half `1`'s and half `0`'s), it is necessary to bias the search process towards smaller subsets. Therefore, the objective in CHC is to minimize the sum of training errors and selected features. Without this "penalty", CHC finds much larger subsets with approximately the same training accuracy [GW98]. Naturally, the overall goal is still to minimize the number of classification errors during final testing.

10.7.2 Results: CF/RSC vs. CHC

Compared to CHC[1], the feature subsets found by CF/RSC perform better during final testing. (See Table 10.3.) The CF/RSC subsets are also smaller than the CHC subsets. Since the time to train an EDT classifier grows approximately with the square of the

1. The CHC experiments were performed by César Guerra-Salcedo.

number of features, CF/RSC is also faster than CHC. On average, CF/RSC takes 50% less time than CHC to evaluate 15,000 solutions.

On the DNA and Cloud data sets, the smaller CF/RSC feature subsets perform significantly worse during training, but they perform better during testing. (See Table 10.4.) Since CF/RSC starts with no features and builds up, it stops in local minima with fewer features. Conversely, CHC starts with many features and works down, so it finds local minima with more features. Since these additional features are at best weakly relevant, they likely cause the search process to over-fit the training data.

Table 10.4: T-tests -- are the CF/RSC and CHC results different?

Data Set	Training	Testing
LandSat	Yes	No
DNA	Yes	Yes
Cloud	Yes	No

10.8 Traditional Feature Selection Techniques

Two basic search procedures for feature subset selection are forward selection and backward elimination. Since backward elimination is computationally impractical for large feature spaces [Koh95], only forward selection is implemented. Truncating the search after the expected number of relevant features have been added, forward selection performs better than CHC on all of the data sets. However, CF/RSC is still slightly better on the two largest data sets (DNA and Cloud).

10.8.1 Forward Selection

Starting with an initial solution of all `0`'s, forward selection finds the best subset with a single feature. At each subsequent step, the best subset which consists of the previous subset and one additional feature is found. Forward selection terminates when all features are included in the subset, and it returns the best subset found along the way (i.e. unlike bit climbing, it does not stop in the first local minimum).

The computational effort required to train a classifier increases with the number of selected features. However, CF/RSC never returns a final subset with more than 18 features. To improve the computational efficiency of forward selection, search is truncated after the first 20 features[1]. The resulting method is called Forward-20.

10.8.2 Results: CF/RSC vs. Forward-20

Compared to Forward-20, CF/RSC performs just slightly better on the two largest data sets (DNA and Cloud)[2]. (See Table 10.5.) Since Forward-20 evaluates much fewer than 15,000 solutions, it is significantly faster than CF/RSC. However, Forward-20 has leveraged the previous results of CF/RSC--it truncates search after 20 features. If complete forward selection is run, more time would be required. Although complete forward selection can be highly effective, greater computational efficiency is often desired.

Table 10.5: Results for CF/RSC (5, 10-90) and Forward-20 on LandSat, DNA, and Cloud data sets. Best, worst, and average values are for 30 independent trials.

		Train				Test		
Data Set	Algorithm	errors			avg. subset size	errors		
		best	worst	avg.		best	worst	avg.
LandSat	CF/RSC	54	93	75.1	12.8	205	313	247.7
	Forward-20	65	96	81.6	15.7	215	281	239.2
DNA	CF/RSC	45	72	57.4	8.5	**74**	142	**104.1**
	Forward-20	45	72	57.6	9.7	79	133	106.4
Cloud	CF/RSC	90	119	102.7	14.0	**101.9**	141.0	**124.7**
	Forward-20	83	122	107.3	14.1	110.8	149.9	131.9

10.9 Discussion

Common Features/Random Sample Climbing is a non-standard crossover operator that has been developed for feature subset selection. Its experimental results can be examined

1. this alteration does not help backward elimination--the final steps with small feature subsets require negligible computational effort.
2. Compared to CHC, Forward-20 performs better on all three data sets.

with respect to standard GAs, the ES-based RSC operator, and machine learning concepts. In general, the explicit identification of the strongly relevant features appears to provide an advantage.

10.9.1 Genetic Algorithms

The utility of the Commonality-Based Crossover Framework is demonstrated on a standard representation. To develop a commonality-based operator, the critical building blocks must be explicitly identified--an analysis that has been omitted in previous applications with standard representations (e.g. [VdJ93]). For feature subset selection, the selected features are useful building blocks, but the unselected features are not. The Common Features/Random Sample Climbing heuristic operator focuses on these critical building blocks better than standard crossover operators.

10.9.2 Restarts, Local Search, and Hybrid Operators

For deterministic hill-climbing procedures (i.e. local optimizers), restarts allow fair time-based comparisons with other (non-deterministic) methods. In particular, these techniques have benefited from commonality-based restarts (see chapter 7). Comparing the results for CF/RSC and RSC alone, it appears that (stochastic/probabilistic) local search methods (e.g. simulated annealing and tabu search) can also benefit from commonality-based restarts. These restarts should eliminate the time required to backtrack out of local minima. Although it still takes time to bring a random solution into the near-optimal region [UPvL91], commonality-based restarts will be more efficient if the restart solution is already in the near-optimal region (see chapter 7).

10.9.3 Machine Learning

It is desirable to train classifiers with small feature subsets. In addition to speed, intuitive interpretations of the data are easier [Koh95]. Comparing the results of CF/RSC and CHC, another advantage is suggested: greater accuracy. The smaller subsets of CF/RSC perform worse in training, but better in testing. Large feature subsets (like those found by CHC) may cause the training data to be over-fitted. Specifically, the selection of additional (weakly relevant) features may induce the classifier to identify subtle characteristics of the training instances.

10.10 Summary

A heuristic (non-standard) operator has been developed for feature subset selection--a standard representation problem. In experiments, Common Features/Random Sample Climbing performs better than standard GAs (e.g. GENESIS and CHC). The new operator focuses on the superior common components that have been identified through an explicit building block analysis. Overall, these results demonstrate that the utility of the commonality hypothesis and the Commonality-Based Crossover Framework extend to standard representations.

Chapter 11

Transmission, Combination, and Heuristic Operators

Transmission is a weak heuristic. If the existing domain-independent design models are extended to heuristic operators, the effectiveness of the embedded construction heuristic can be handicapped by transmission.

11.1 Overview

The Commonality-Based Crossover Framework addresses heuristic operators directly--it is not a domain-independent model that has been extended to this operator category. From its perspective, the traditional mechanisms of domain-independent operators (i.e. transmission and combination [Rad91]) are merely default heuristics--they should be *replaced altogether* when stronger, problem specific heuristics are available. Unfortunately, through the historical perception that combination is the critical aspect of crossover, these domain-independent models still influence the design of heuristic operators[1]. For example, Greedy Crossover (see section 5.2.1) is a heuristic operator that places the transmission and combination "heuristics" ahead of the problem specific Nearest Neighbor heuristic.

The results of Greedy Crossover suggest that transmission and combination are not strong heuristics. To examine this hypothesis, these mechanisms have been imposed upon two commonality-based heuristic operators. Specifically, Maximum Partial Order/Arbitrary Insertion (MPO/AI) and Common Features/Random Sample Climbing (CF/RSC) have been modified to obey strict transmission. In the converted operators, the offspring search space is defined by the (feasible) combinations of parent schemata. This restriction handicaps the effectiveness of the embedded construction heuristic.

The "convergence" in Convergence Controlled Variation is caused by transmission--the current search space is limited to parent genes. For better or worse, heuristics also apply implicit limits to their search space (see section 6.3.4). Since the inclusion of both limits can be redundant, the Commonality-Based Crossover Framework suggests that only the heuristic should control variation. With the superior performance of these heuristic operators, the role of transmission and combination in heuristic operators is cast into doubt.

11.2 Heuristic Operators in Convergence Controlled Variation

In the (domain-independent) model of Convergence Controlled Variation (CCV) [EMS96], the offspring search space is defined by transmission--offspring must be *combi-*

1. Before components can be combined, they must be transmitted.

nations of the parent genes (see section 2.5.2). Traditionally, crossover (recombination) is used to sample this search space randomly. Conversely, this search space can be explored with problem specific heuristics.

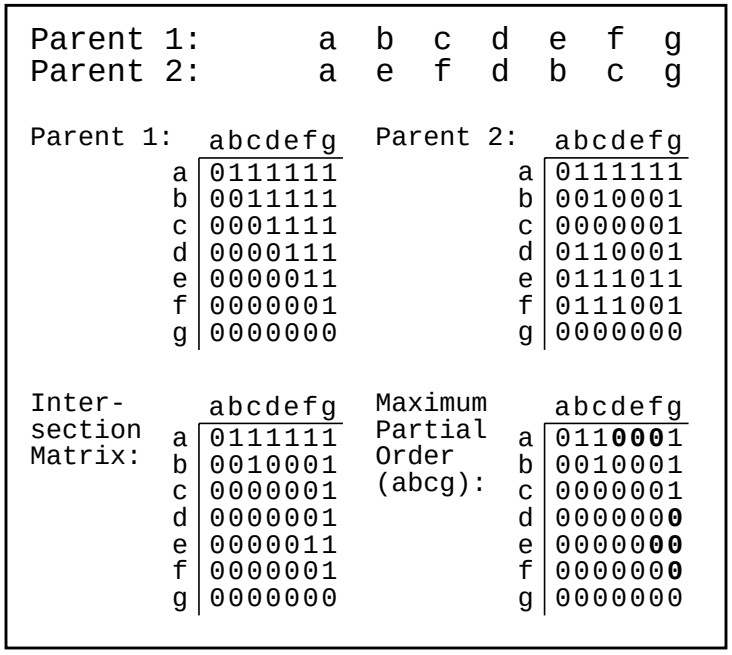
Starting from the maximal common schema, construction heuristics can be incorporated into Convergence Controlled Variation by following the two-step process of the Commonality-Based Crossover Framework. If strict transmission is imposed onto the construction heuristic, the offspring solutions will stay within the search space defined by CCV. This heuristic model for Convergence Controlled Variation isolates the effects of transmission.

11.3 The Traveling Salesman Problem

Maximum Partial Order/Arbitrary Insertion is a commonality-based heuristic operator that has been developed for the Traveling Salesman Problem (see section 5.3.2). When transmission of all precedence relationships is enforced, it is converted into Matrix Intersection/Arbitrary Insertion (MI/AI). Experimental results show that MI/AI performs worse than MPO/AI. The additional precedence constraints imposed by transmission handicap the effectiveness of Arbitrary Insertion.

11.3.1 Matrix Intersection/Arbitrary Insertion

To develop the Maximum Partial Order of two parent solutions, their sequences are converted into Boolean matrices, the matrices are intersected, and a partial order graph is generated. When the Maximum Partial Order is extracted from the partial order graph, some arcs are ignored (e.g. `e` to `f`--see Figure 5.4). Thus, the Boolean matrix which represents the MPO specifies fewer precedence relationships than the intersection matrix. (See Figure 11.1.) Unlike partial orders, the omission of these precedence relationships violates the principle of transmission for order-based schemata.



Parent 1	a	b	c	d	e	f	g
a	0	1	1	1	1	1	1
b	0	0	1	1	1	1	1
c	0	0	0	1	1	1	1
d	0	0	0	0	1	1	1
e	0	0	0	0	0	1	1
f	0	0	0	0	0	0	1
g	0	0	0	0	0	0	0

Parent 2	a	b	c	d	e	f	g
a	0	1	1	1	1	1	1
b	0	0	1	0	0	0	1
c	0	0	0	0	0	0	1
d	0	1	1	0	0	0	1
e	0	1	1	1	0	1	1
f	0	1	1	1	0	0	1
g	0	0	0	0	0	0	0

Inter-section Matrix	a	b	c	d	e	f	g
a	0	1	1	1	1	1	1
b	0	0	1	0	0	0	1
c	0	0	0	0	0	0	1
d	0	0	0	0	0	0	1
e	0	0	0	0	0	1	1
f	0	0	0	0	0	0	1
g	0	0	0	0	0	0	0

Maximum Partial Order (abcg)	a	b	c	d	e	f	g
a	0	1	1	**0**	**0**	**0**	1
b	0	0	1	0	0	0	1
c	0	0	0	0	0	0	1
d	0	0	0	0	0	0	**0**
e	0	0	0	0	0	**0**	**0**
f	0	0	0	0	0	0	**0**
g	0	0	0	0	0	0	0

Figure 11.1: Comparison of Matrix Intersection and Maximum Partial Order.

The Matrix Intersection (MI) operator (see section 4.2.3) preserves all of the (common) precedence relationships. Since it follows Radcliffe's design principles (i.e. respect, transmission, and assortment [Rad91]), MI is a viable operator for domain-independent Convergence Controlled Variation. To convert MI into a heuristic operator, Arbitrary Insertion can explore the offspring search space (i.e. generate the remaining precedence relationships). Equivalently, the additional precedence constraints of the intersection matrix can be super-imposed onto MPO/AI. From either perspective, the resulting heuristic operator is Matrix Intersection/Arbitrary Insertion[1].

11.3.2 Results: MPO/AI vs. MI/AI

To allow direct comparisons with MPO/AI, the Matrix Intersection/Arbitrary Insertion experiments use a population size of 400, and it is seeded with convex hull/Arbitrary Insertion solutions. From this population, the parents for MI/AI are both selected by 2-tournament--the additional selection pressure helps Matrix Intersection/Arbitrary Insertion. Regardless, MPO/AI performs better than MI/AI. (See Table 11.1.)

1. The starting sub-tour is again the Maximum Partial Order. However, Arbitrary Insertion is modified to preserve the additional precedence constraints in the intersection matrix.

Table 11.1: Comparison of MPO/AI and MI/AI on 5 TSP instances. Results are for a steady-state GA with a population of 400 run until 10 generations pass without an improvement. Values are percent distance from known optimum for average of 5 runs. Experiment runtimes are given for a SPARC 20.

TSP Instance	Average Best CH/AI Start	Average Best MPO/AI	Runtime (min)	Average Best MI/AI	Runtime (min)
d198	+ 3.05 %	+ 0.95 %	3	+ 1.14 %	4
lin318	+ 6.04 %	+ 0.63 %	13	+ 1.42 %	15
fl417	+ 1.91 %	+ 0.57 %	15	+ 0.61 %	18
pcb442	+ 8.97 %	+ 1.84 %	37	+ 3.18 %	47
u574	+ 8.45 %	+ 2.20 %	74	+ 2.63 %	73
average	+ 5.68 %	+ 1.24 %		+ 1.80 %	

The MPO/AI and MI/AI operators only differ by the inclusion of strict transmission in Matrix Intersection/Arbitrary Insertion. The precedence relationships which MPO ignores in the intersection matrix can be coincidental. (See Figure 11.2.) Subsequently, their enforcement by transmission may interfere with the performance of AI. Arbitrary Insertion is a strong, problem specific heuristic which (compared to transmission) can identify better (order-based) schemata for the TSP.

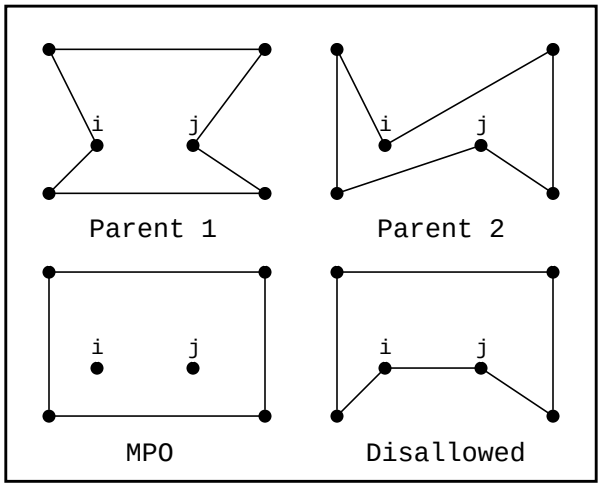


Figure 11.2: Example of a coincidental precedence relationship. Although city `i` precedes city `j` in both parents, the construction heuristic may prefer to place city `j` before city `i`.

11.4 Feature Subset Selection

Common Features/Random Sample Climbing is the commonality-based heuristic operator that has been developed for feature subset selection (see section 10.5). When transmission of 0's is imposed upon CF/RSC, the resulting operator is Convergence Controlled Variation/Random Sample Climbing (CCV/RSC). Experimental results show that CCV/RSC performs worse than CF/RSC. When it is required that features which are not selected in either parent (i.e. their common 0's) cannot appear in the offspring, the effectiveness of Random Sample Climbing is handicapped.

11.4.1 Convergence Controlled Variation/Random Sample Climbing

Feature subset selection is a standard representation problem. Since standard crossover operators preserve all of the common 1's and all of the common 0's (i.e. they obey strict transmission), the "variations" available in the offspring search space are due to the uncommon bits/genes. Convergence Controlled Variation suggests that crossover operators should be limited to this search space.

To allow direct comparisons with CF/RSC, Random Sample Climbing has been used to explore the offspring search space defined by Convergence Controlled Variation. Starting from the partial solution of Common Features, the resulting heuristic operator is Convergence Controlled Variation/Random Sample Climbing. Equivalently, this operator is also developed by super-imposing the transmission of 0's onto CF/RSC and by disallowing RSC to back-track common 1's. From either perspective, the search space in CCV/RSC is limited to the allele positions represented by uncommon bits in the parents.

11.4.2 Results: CF/RSC vs. CCV/RSC

The Convergence Controlled Variation/Random Sample Climbing heuristic operator has been applied to the LandSat data set, the DNA data set, and the Cloud Data set. In these experiments, n and λ are again treated as control variables (set to 3 and 30 respectively). To match the parameters of CF/RSC (5, 10-90), k is set to 5, the population size is set to 10, and 90 offspring solutions (15,000 total evaluations) are allowed. Using the same GENITOR set-up (i.e. 1.00 selection bias and duplicate solutions disallowed), CCV/RSC is less effective than CF/RSC. (See Table 11.2.)

Table 11.2: Results for CF/RSC (5, 10-90) and CCV/RSC on LandSat, DNA, and Cloud data sets. Best, worst, and average values are for 30 independent trials.

				Train				Test		
Data Set	k	RSC	CCV/ RSC	errors			avg. subset size	errors		
				best	worst	avg.		best	worst	avg.
LandSat	5	10	90	57	97	78.4	11.6	228	282	249.6
	5	20	80	55	94	76.4	11.6	230	315	253.9
	CF/RSC			**54**	93	**75.1**	12.8	**205**	313	**247.7**
DNA	5	10	90	55	82	68.2	7.6	93	167	123.4
	5	20	80	51	76	61.8	8.2	86	128	107.3
	CF/RSC			**45**	72	**57.4**	8.5	**74**	142	**104.1**
Cloud	5	10	90	95	128	110.4	9.3	120.1	156.4	134.9
	5	20	80	94	123	107.1	9.9	117.0	151.4	132.0
	CF/RSC			**90**	119	**102.7**	14.0	**101.9**	141.0	**124.7**

The principle of strict transmission handicaps the ability of Random Sample Climbing to assemble the best weakly relevant features. In particular, a desired feature (1) may be absent from the entire population (i.e. the population may not have enough diversity). This situation is partially rectified by increasing the population size to 20, but CF/RSC still performs better. Overall, transmission has not improved the performance of Random Sample Climbing.

11.5 Discussion

The domain-independent design principle of transmission has been super-imposed upon two previously developed heuristic operators. Although combination has been viewed as a critical feature of crossover (see section 2.4.3), limiting the offspring of heuristic operators combinations of their parent genes is not always productive. Specifically, MI/AI performs worse than MPO/AI on the TSP, and CCV/RSC performs worse than CF/RSC in feature subset selection.

Although the commonality-based heuristic operators perform better than their corresponding versions based on Convergence Controlled Variation, they still have inefficiencies. For example, MPO/AI suffers from negative heuristic amplification (see Figure

6.4), and CF/RSC will repeatedly reexamine irrelevant features. There is too little diversity in the search space of MPO/AI, and there is too much diversity in the search space of CF/RSC.

The ideal balance point between diversity and focus is difficult to estimate. Although search space reductions (which magnify the convergence effects of transmission) improve the performance of blind operators (see chapter 9), transmission itself impairs the performance of heuristic operators. Conversely, search space reductions (e.g. starting MPO/AI from the convex hull) have improved the performance of heuristic operators. Each problem domain must be examined individually.

11.6 Summary

Transmission and combination are traditionally seen as the primary mechanisms of crossover. However, when these features were imposed upon heuristic operators, they have handicapped the effectiveness of the embedded construction heuristic. For the development of heuristic operators, it should be more productive to use the Commonality-Based Crossover Framework than to extend the existing domain-independent design models.

Chapter 12

Conclusions

For iterative improvement to be more successful than random search, existing candidate solutions should facilitate the discovery of better candidate solutions. Essentially, good solutions must share exploitable features. The explicit identification of these common components leads to an alternative approach for iterative improvement. Instead of changing (bad) parts in (single) candidate solutions, good parts can be preserved from two candidate solutions.

Pursuing this alternative approach in genetic algorithms, the commonality hypothesis suggests that schemata common to above-average solutions are above average. These common components represent the good parts that should be preserved. Subsequently, the Commonality-Based Crossover Framework redefines crossover as a two step process: 1) preserve the maximal common schema of two parents, and 2) complete the solution with a construction heuristic.

To balance the exploitation of common components with the necessary exploration for new components, diversity is required. The construction heuristic is responsible to generate diversity (random errors versus systematic errors) and a population of solutions allows this diversity to be distributed (different parent pairs can have different common components). Without enough diversity, undesirable components can become common, and the final solution will be sub-optimal.

The broad utility of the new design model has been demonstrated through the development of domain-independent operators, heuristic operators, and hybrid operators for benchmark and practical problems with standard and non-standard representations. Although most results are relative, the commonality-based operators consistently perform better than comparable operators which emphasize combination. Experimental evidence indicates that components common to above-average parents can have a measurable, superior relative fitness. In these cases, the uncommon components targeted by combination will have a below-average fitness relative to their parents.

Selection chooses components for exploitation. Therefore, the preservation of common components is a form of selection--these components are exploited. This commonality-based form of selection has been isolated in GENIE (a GA that eliminates fitness-based selection at the individual level). Since the effectiveness of heuristic operators can be

amplified by commonality-based restarts, the productive value of commonality-based selection corroborates the commonality hypothesis. The common schemata it preserved were above average.

Although commonality-based selection was first isolated in heuristic operators, its effects can be transferred back to standard (domain-independent) operators. The preservation of (above-average) common components restricts changes to the (below-average) uncommon components of the parents. The probability that these changes are beneficial should increase with this focus. Since multiple parents are required to identify common components, commonality-based selection is an advantage that multi-parent operators (e.g. crossover) can have over single-parent operators (e.g. mutation).

Chapter 13

Extensions and Future Work

A series of extensions and open issues are suggested for the Commonality-Based Crossover Framework and the commonality hypothesis.

13.1 Interactive Search Space Reductions

Search space reductions can be specified interactively. Although a global parameter was used for flow shop scheduling (see chapter 9), it does not preclude the addition or deletion of individual constraints. For example, a graphic user interface (GUI) has been developed for Common Clusters/Insertion (see section 8.4) to allow the initial customer clusters to be set manually[1]. A GUI allows unique and/or ill-defined constraints to be added as necessary (in real-time). Since real world problems often include similar operations-level preferences/constraints, interactive search space reductions may be useful in practical environments.

13.2 Practical Heuristic Amplification

Through the effects of heuristic amplification (see section 6.3), commonality-based restarts of a good construction heuristic will be more effective than random restarts. To demonstrate the full value of commonality-based selection and heuristic amplification, a relevant problem that is currently solved by random restarts is required. Unfortunately, stand-alone construction heuristics rarely provide the best optimization technique. A suitable domain has yet to be found.

13.3 Theoretical Heuristic Amplification

A commonality-based heuristic operator that encapsulates an ideal construction heuristic will converge to the optimal solution. The derivation of the previous statement is independent of problem size (see section 3.7.2). Therefore, convergence occurs in a *constant* number of generations. In the (unlikely) event that a polynomial-time ideal construction heuristic can be developed, it will solve NP-complete problems in polynomial time.

1. In this system, interactive results were better than random initial clusters, but they were still worse than tabu search. However, this study was uncontrolled--the user had knowledge of the best-known solutions.

13.4 Open-Loop Optimization

The existence of heuristic amplification leads to the concept of open-loop optimization. Unfortunately, it is difficult to imagine a practical application where open-loop optimization will be successful. In particular, heuristic amplification is based on construction heuristics which require local evaluation information. However, open-loop optimization is only viable when global evaluations are too expensive[1]. Since global payoff is often a summation of local cost functions, it may be difficult to resolve this contradiction. A problem domain with good construction heuristics and an expensive overall evaluation function is required to test the practical value of open-loop optimization.

13.5 Lamarckian Learning

Open-loop optimization resembles Lamarckian evolution. Fitness-based feedback is not required because the heuristic provides "a built-in drive toward perfection of adaptations". Since a learning algorithm acts like a construction heuristic (it builds a world view incrementally), the Commonality-Based Crossover Framework may be a useful model for agent-based learning systems.

13.6 Commonality-Based Random Hill Climbing

In random hill climbing (see section 2.8.1), the first improving solution is taken. Compared to (complete) hill climbing, random hill climbing can be more efficient and just as effective. However, in problem domains with large operator sets, the improving moves eventually become scarce, and the relative efficiency will degrade. To increase the efficiency, it is desirable to identify the improving operators.

Hill climbing operators act on a single solution--just like mutation. However, the probability of a beneficial mutation is expected to increase when mutation is restricted to uncommon bits (see section 3.8). By extension, hill climbing operators that target uncommon components[2] may cause improvements more often[3]. When these operators

1. The removal of evaluations is expected to improve computational efficiency only. For the same number of crossover applications, fitness-based selection should still improve solution quality (see section 6.3.5).

are applied first, the resulting procedure becomes “commonality-based random hill climbing”. This modification can be applied to any point-search method (e.g. simulated annealing and tabu search).

13.7 Machine Learning

Many techniques in artificial intelligence implicitly seek to identify the common components. For example, incremental learning methods (e.g. clustering, neural nets, reinforcement learning, etc) find the common core by “cancelling out” the differences in the individual instances. When it is not productive to keep common components (e.g. common `0`’s in feature subset selection), these methods may not function properly. The commonality hypothesis provides an explicit test to examine these implicit actions.

13.8 Case Studies

Case studies (e.g. in business school) are often presented one at a time. The natural tendency is to look for things that went wrong--things that can be improved. However, it can be just as useful to know what went right--what should be repeated. If two cases are studied at the same time, the commonality hypothesis suggests that their common components will represent things that should be repeated.

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2. An (unspecified) benchmark solution is required to help identify common components.
3. Trivially, if mutation on a `n`-bit binary string is converted into `n` “mutate-bit” operators, the previous argument transfers directly see section 3.8).

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