Exterior Path Relinking for Zero-One Optimization

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Abstract: Path relinking (PR) maintains a reference set of elite and diverse solutions, and generates new solutions between and beyond *initiating* and *guiding* solutions selected from this set as a foundation for an evolutionary solution process. However, in spite of the widespread application of path relinking in combinatorial optimization, almost all PR implementations only consider the *between-form* of PR. This note discusses the *beyond-form* of path relinking, which we call *Exterior Path Relinking*, and focuses on its relevance for diversification strategies in binary optimization. Finally, we also observe how to combine the Exterior (beyond) and Interior (between) forms of path relinking.

1. Introduction

Path relinking (PR) creates *combinations* of solutions by a process of generating paths between selected points in neighborhood space. The approach, as first suggested in Glover (1989) and then formalized and given the path relinking name in Glover and Laguna (1993), takes advantage of the path interpretation of solution combinations as a foundation for numerous applications in combinatorial optimization, as illustrated in the work of Reeves and Yamada (1998), Laguna and Marti (1999), Laguna and Marti (2003), Piñana et al. (2004), Ghamlouche, Crainic, and Gendreau (2004), James, Rego and Glover (2005), Glover, Ho and Gendreau (2006), Zhang and Lai (2006), Yagiura, Ibaraki and Glover (2006), Yagiura et al. (2007), Resende et al. (2010), Vallada and Ruiz (2010), Marti et al. (2011), Marinakis and Marinaki (2012), Ribeiro and Resende (2012), Wang et al. (2012), Marti and Sandoy (2012), Lai et al. (2013), Duarte, Martí and Gortazar (2013), Rahimi-Vahed et al. (2013), and Marti, Resende and Ribeiro (2013).

However, the principles of path relinking are somewhat broader than those employed in most of its implementations, and offer strategies for combinatorial and non-linear optimization that have not been fully examined. To clarify these aspects of PR we begin by reviewing a few observations from Glover (1996) that express the basic themes of path relinking and at the same time highlight the relevance of strategies that to date remain unexplored.

> The character of paths generated by PR is easily specified by reference to attribute-based memory, as used in tabu search. In particular, it is only necessary to select moves in a neighborhood space that perform the following simple function: upon starting from an *initiating solution*, the moves must progressively introduce attributes contributed by a *guiding solution* (or reduce the distance between attributes of the initiating and guiding solutions). The process invites variation by interchanging the roles of the initiating and guiding solutions, inducing each to move simultaneously toward the other as a way of generating combinations. (When the goal for combining the solutions can be expressed as an optimization model, algorithmic processes may appropriately be incorporated to generate the moves.)

By curious coincidence, this preliminary portrayal of path relinking embodies notions that somehow were overlooked in a large number of PR implementations that followed. For example, the ideas of interchanging initiating and guiding solutions, and of progressing simultaneously from each of these solutions toward the other, failed to receive attention in early PR investigations and were finally "reinvented" a number of years after they were initially proposed. However, the chief observation that motivates the present note concerns the relevance of paths that go beyond the initiating and guiding solutions, and hence create the basis for

what we call *Exterior Path Relinking*.[1] This element is broached in the same article as follows.

> The scope of strategies made available by path relinking is significantly affected by the fact that the term *neighborhood* has a broader meaning in tabu search than it typically receives in the popular literature on search methods. Often, the neighborhood terminology refers solely to methods that progressively transform one solution into another. Such neighborhoods are called *transition neighborhoods* in tabu search, and are considered as merely one component of a collection of neighborhoods that also include *constructive* and *destructive neighborhoods*.

The article elaborates on this to highlight the feature of PR that underlies the main preoccupation of the present work.

> In addition, tabu search characteristically endows such a collection of neighborhoods with the ability to operate in regions beyond those visited by standard procedures for generating solutions. Strategic oscillation approaches in TS, for example, include variations that build solutions beyond the point of "complete construction," and more generally introduce complementary constructive and destructive processes that go beyond standard boundaries in both directions. By selecting neighborhoods that are relevant to a given problem setting, drawing on this expanded interpretation of a neighborhood, path relinking automatically provides solution combination procedures that are appropriate for specific contexts.[2]

From this starting point, we focus specifically on the case of binary optimization and consider the manner in which the PR framework usefully specializes to the setting where solutions consist of vectors of zero-one variables.

2. The Structure of Exterior Path Relinking for Binary Optimization

Introducing a minimum of notation to keep the description simple, the essence of Exterior PR for binary optimization can be characterized as follows.

Let x^I and x^G respectively denote an initiating and guiding solution drawn from a Reference Set R of n-dimensional binary vectors x in a feasible space. We begin by examining a path relinking process that is launched from x^I and progresses in the direction of x^G. Instead of stopping at x^G, we are concerned with the exterior portion of the path that begins at x^G, and then assigns new values to components of x^G to yield a succession of vectors that do not return in the direction of x^I.

This is accomplished, starting with $x = x^G$, as follows. Let $J = \{j: x_j^G = x_j^I\}$ and $J^{\sim} = \{j: x_j^I \neq x_j^G\}$ (hence $|J| + |J^{\sim}| = n$). We focus on changing the value of only those components x_j

[1] The first discussion of Exterior Path Relinking appears in Glover and Laguna (1993), where it is called Extrapolated Path Relinking.
[2] This aspect may be contrasted with the organization of genetic algorithms, where each new class of problems initiates a search for "new crossovers" in order to overcome the limitations of classical models derived from the genetic metaphor.

for $j \in J$, due to the fact that if we were to change the value of x_j for some $j \in J^{\sim}$ we would move either in the direction of x^I or x^G, contrary to the goal of the exterior form of PR. Instead of starting with $x = x^G$, we could also start the Exterior PR procedure from the vector x that was selected as best during an Interior Path Relinking process, yielding x "between" x^I and x^G.

By employing aspiration criteria that allow the path to deviate to visit high quality neighbor solutions, or by invoking rules that induce the process to skirt infeasibilities, the strict requirement of selecting x_j for $j \in J$ may be relaxed. However, any such move that flips the value of x_j for some $j \in J^{\sim}$ must ultimately be reversed unless the relinking process is terminated (and the resulting x vector is then included among those that are submitted to a solution improvement process, which may also be designed to eliminate infeasibilities).

To summarize then, subject to the noted exceptions, Exterior PR chooses a variable x_j for $j \in J$ and flips it (changes its value to $1 - x_j$) to yield the next x vector in the process. A candidate list rule following Glover and Laguna (1997) may be employed that restricts attention to a circumscribed subset of J in the case where J is large.

3. Choice Rules and Features of the Exterior PR Process.

The variable x_j for $j \in J$ that is selected to be flipped at each stage of the exterior PR process will typically be one that produces a new solution x with the highest evaluation (best objective function value) from the accessible candidates. In this manner the search is drawn toward attractive solutions (and potential improving sequences) when these are available. However, in some instances a less aggressive strategy that selects x_j by using ideas of probabilistic tabu search (or even randomly) can be useful, provided the same pair of initiating and guiding solutions is used multiple times. The path can terminate after finding a solution that improves on the best of x^I or x^G (should this occur) or after a minimum specified number of steps (to ensure diversification), provided an estimate indicates that a better solution is unlikely to be found by going farther.

Such an estimate may, for instance, make use of the evaluation of the final solution x^F on the exterior path, which results by flipping all variables x_j for $j \in J$ (e.g., immediately performing this operation when starting from $x = x^G$ to identify x^F). At any juncture of generating the exterior path, if x^F should appear more attractive than the current x, the method can elect to jump immediately from x to x^F and work backward toward the solution that initiated the jump. The option of progressing from both ends toward the middle likewise arises by analogy to the corresponding strategy of the original PR proposal.

In this exterior form of PR it is natural to choose x^G to have a higher evaluation than x^I. For example, x^G might always be selected to be the current best solution found (or one of the few best solutions found), and x^I may range over a subset of solutions in the reference set R that are chosen to be diverse in relation to x^G and each other.

As underscored in the tabu search literature, diversification should not be divorced from intensification, but should aim at producing high quality solutions at the same time that it drives the solution process into new regions. The exterior form of path relinking is usefully structured to accomplish this.

4. Inside-Out Variants

We call attention to another form of interior path relinking, which we call Inside-Out Relinking, which can also be used with Exterior Path Relinking and in addition can be adapted to provide variants of Exterior PR. The Inside-Out Relinking approaches come in two guises, *fractional* and *discrete*.

Fractional Inside-Out Relinking:

The early path relinking literature also proposed selecting more than one guiding solution and to choose moves that introduce attributes contained in at least one of these solutions but not in the current solution. Choices made along the way can be locked in permanently or temporarily using tabu restrictions, until reaching a desired cutoff.

An interesting (and effective) form of this approach in Lu, Glover and Hao (2010), which we will call Fractional Inside-Out Relinking, begins by selecting two solutions x' and x'' from the Reference Set R, both of which are to be treated as guiding solutions (hence they may also be represented as x^{G1} and x^{G2}). Then the initiating solution is chosen to be the midpoint of x' and x'' (a point commonly selected by Scatter Search); i.e.,

$$x^I = 0.5(x' + x'')$$

This yields $x_j^I = 0.5$ if $x_j' \neq x_j''$, and hence moving from x^I toward the guiding solutions will consist at each step of replacing the value of some fractional component of the current solution x, starting from $x = x^I$, with a value of 0 or 1.

By extending our previous definition of $J = \{j: x_j^G = x_j^I\}$ to account for having both x' and x'' as guiding solutions in place of a single guiding solution x^G, we may write $J = \{j: x_j' = x_j'' = x_j^I\}$, which in this case is the same as $J = \{j: x_j' = x_j''\}$. Hence, the complement of J is again given by $J^{\sim} = \{j: x_j^I \neq x_j^G\}$ and we have $x_j^I = 0.5$ for $j \in J^{\sim}$. Consequently, as in customary Interior PR approaches we focus on changing values of variables x_j for $j \in J^{\sim}$.

In this Fractional Inside-Out relinking strategy, each 0 or 1 value assigned to some x_j for $j \in J^{\sim}$ is permanently fixed, and the choice rule alternates by setting $x_j = x_j'$ on odd steps and $x_j = x_j''$ on even steps, so that ultimately x' and x'' each contribute approximately an equal number of their values to x. The purpose of this strategy is to make the final x as diverse as possible in relation to x' and x'', subject to lying between these solutions.

An evident variation on this approach is to allow either of the two types of assignments $x_j = x_j'$ or $x_j = x_j''$ to be made on a given step according to which yields the highest evaluation, subject to the condition that a particular type of assignment is only permitted to be made for at most s steps, where $s = |J^{\sim}|/2$ (rounded). Giving s a larger value such as $s = (3/4)|J^{\sim}|$ would allow the method to adaptively choose a given type of assignment between $(1/4)|J^{\sim}|$ and $(3/4)|J^{\sim}|$ times.

Discrete Inside-Out Relinking:

We observe that it would be possible to achieve the "diversity effect" produced by Fractional Inside-Out Relinking if a customary interior path relinking approach were used, choosing either x' or x'' as an initiating solution x^I and the other as a guiding solution x^G, and then stopping the relinking process when reaching a point halfway between them. We could similarly achieve an adaptive effect by requiring the number of flips performed, starting with $x = x^I$, to lie between lower and upper bounds L and U, where for symmetry $U = |J^{\sim}| - L$, so that solutions permitted to be selected lie at a Hamming distance of at least L from both x^I and x^G. (Interior PR approaches normally choose an L value that is relatively small, with the intent of being just large enough to prevent an acceptable solution from lying too close to a path endpoint, rather than to enforce diversity.) However, it is important to note that this modified form of a customary Interior Relinking approach is not equivalent to a Fractional Inside-Out approach, since each step of the fractional procedure involves changing a value of $x_j = 0.5$ to a value $x_j = 0$ or 1 and hence the evaluation to identify a best move at each step will differ from that employed by a process in which every x_j has an integer value throughout.

Building on this observation, we can use the design of the Fractional Inside-Out approach more directly to formulate analogous Discrete Inside-Out Path Relinking approaches. For this, we select solutions x^I and x^G as in a customary Interior Path Relinking method, and then immediately move from x^I to a "midpoint" solution x^M by flipping half the variables in the set $J^{\sim} = \{j: x_j^I \neq x_j^G\}$. Such a step could randomly select the variables to flip or could elect to flip $|J^{\sim}|/2$ variables that have either the best or the worst evaluations relative to x^I. Once x^M is thus identified we create two paths, one using the pair (x^M, x^I) to give the initiating and guiding solutions and the other using the pair (x^M, x^G) to give the initiating and guiding solutions. For each of these paths we enforce the restriction that the acceptable solutions lie no closer than L flips from either x^I or x^G. Subject to this condition, the initiating and guiding roles of a given pair can be interchanged.

5. Combining Interior and Exterior Path Relinking

Interior Path Relinking, including the Fractional and Discrete Inside-Out approaches, can be combined with Exterior Path Relinking framework in several ways. The simplest approach is to stipulate that the starting solution x for the exterior process is the one selected as best from the Interior PR process. In the fractional case we note that "best" includes the provision that all variables have finally been assigned 0-1 values.

Natural variants can be created by employing the version of path relinking that makes use of multiple guiding solutions. One form of such variants can form the Interior approach by treating the intersection of the guiding solutions and the initiating solution as an incomplete base solution, and then using a constructive solution process to determine the values of remaining variables, whereon the final complete solution is used as the solution for launching the Exterior PR process.

6. Conclusions

The simple framework of Exterior Path Relinking for zero-one optimization is easy to program and test. The framework can be directly incorporated to supplement methods that use more customary Interior Path Relinking strategies, although we have seen how other interior strategies can also be used. The resulting procedure can then be subjected to experimentation to determine the benefits that may come from joining the interior and exterior approaches. As previously noted, variants introduced for Interior PR can readily be adapted to create analogous variants for Exterior PR strategies. Interesting avenues for exploration are provided by investigating rules that manipulate transitions between phases of Exterior and Interior Path Relinking, applied either separately or in conjunction with each other. It would likewise be worthwhile to identify classes of problems (perhaps as a function of the ruggedness of their landscapes) for which such variants prove most effective.

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Appendix: Vocabulary Building

The tabu search strategy of vocabulary building can be a useful adjunct to Exterior Path Relinking. As noted in Glover (1996), vocabulary building may be conceived as a special instance of path relinking that identifies meaningful fragments of solutions, rather than focusing solely on full vectors, as a basis for generating combinations. A pool of such fragments is progressively enriched and assembled to create larger fragments, until ultimately producing complete trial solutions. In some settings these fragments can be integrated into full solutions by means of optimization models.

Vocabulary building has two key objectives: (1) to identify a good collection of reference points, in this case consisting of “partial solutions” (which include the fragments), and (2) to identify paths in neighborhood space that will unite components of these partial solutions, with suitable attendant modifications, to produce complete solutions. (Again it is important to keep in mind that neighborhood spaces include constructive and destructive spaces, as well as transition spaces. Attributes of different partial solutions may be imperfectly compatible, and hence the synthesis of such partial solutions can benefit from multiple or "compound" transformations to create effective linkages.) As a special instance, of course, solution fragments may be united by linear combinations, as in scatter search.

The crucial element of adaptive memory that permeates these alternative modes of combination, and binds them to other tabu search strategies, affords challenging opportunities for research into the nature and meaning of "intelligent combinations." Additional discussion of vocabulary building in relation to path relinking can be found in Glover, Laguna and Marti (2000).