Title:
Improved Large-Step Markov Chain Variants for the Symmetric TSP

Authors:
Inki Hong, Andrew B. Kahng and Byung-Ro Moon
UCLA Computer Science Department
Los Angeles, CA 90095-1596 USA

Communicating Author:
Andrew B. Kahng
UCLA Computer Science Department
3713 Boelter Hall
Los Angeles, CA 90095-1596 USA
E-mail: abk@cs.ucla.edu
Tel. 310-206-7073 (office), 310-825-7578 (fax)

Abstract: The *large-step Markov chain* (LSMC) approach is the most effective known heuristic for large symmetric TSP instances; cf. recent results of [Martin, Otto and Felten, 1991] and [Johnson, 1990]. In this paper, we examine relationships among (i) the underlying local optimization engine within the LSMC approach, (ii) the "kick move" perturbation that is applied between successive local search descents, and (iii) the resulting LSMC solution quality. We find that the traditional "double-bridge" kick move is not necessarily optimum: stronger local optimization engines (e.g., Lin-Kernighan) are best matched with stronger kick moves. We also propose use of an adaptive temperature schedule to allow escape from deep basins of attraction; the resulting *hierarchical* LSMC variant outperforms traditional LSMC implementations that use uniformly zero temperatures. Finally, a population-based LSMC variant is studied, wherein multiple solution paths can interact to achieve improved solution quality.

Key Words: large-step Markov chain; optimization; simulated annealing; traveling salesman problem

1 Preliminaries

Given a set of cities and a symmetric matrix of all inter-city distances, the symmetric traveling salesman problem (TSP) seeks a shortest tour which visits each city exactly once. The symmetric TSP is NP-hard [Garey and Johnson, 1979], and has been extensively studied both in terms of its combinatorial structure and as a testbed for exact and heuristic methods [Lawler et al., 1985] [Johnson and McGeoch, 1997]. Studies such as [Johnson, 1990] point to greedy local search (e.g., using the fast 3-Opt [Bentley, 1992] or the Lin-Kernighan (LK) [Lin and Kernighan, 1973] neighborhood structure) as the most effective approach for practical instances. Over the past decade, *iterated descent* [Baum, 1986a] [Baum, 1986b] has been shown to be an effective means of applying a given greedy local search "engine": iteratively perform a greedy descent, then perturb the resulting local minimum to obtain the starting solution for the next greedy descent. Currently, the "large-step Markov chain" (LSMC) heuristic of [Martin, Otto and Felten, 1991] and the "iterated LK" heuristic of [Johnson, 1990] are believed to be the best-performing iterated descent variants (and, indeed, the best-performing of all heuristics for obtaining near-optimal solutions [Johnson and McGeoch, 1997]); we generically refer to both of these as LSMC methods.

1.1 Previous Large-Step Markov Chain Implementations

The LSMC approach is described in Figure 1, following the presentation in [Martin, Otto and Felten, 1991]. LSMC alternately applies (i) a (greedy) local optimization procedure *Descent*, followed by (ii) a "kick move" which perturbs the current local minimum solution in order to obtain a starting solution for the next *Descent* application. Local search (i.e., *Descent*) procedures used in previous implementations include LK as well as k-Opt methods.[1] [Martin, Otto and Felten, 1991] used both LK and a fast implementation of 3-Opt; [Johnson, 1990] used LK only. Kick move perturbation of the current local minimum tour is typically achieved using a k'-change, with k' not necessarily equal to k. Both [Martin, Otto and Felten, 1991] and [Johnson, 1990] use random "double-bridge" 4-change kick moves, illustrated in Figure 2. According to [Martin, Otto and Felten, 1991], the double-bridge kick move is chosen for its ability to produce large-scale changes in the current tour without destroying the solution quality via too large a random perturbation. Furthermore, it is a relatively small perturbation whose "non-sequential" structure [Lin and Kernighan, 1973] is not easily reproduced by the Lin-Kernighan algorithm.

As can be seen from Figure 1, the LSMC method actually performs simulated annealing over local minima, with { kick move + *Descent* } as the neighborhood operator. In other words, if a new local minimum has lower cost than its predecessor, it is always adopted as the current solution; otherwise, it is adopted with probability given by the Boltzmann acceptance criterion (cf. Step 2.3 in Figure

[1] Some fairly standard terminology: A k-change operation modifies the current tour by removing up to k existing edges and reconnecting the resulting tour fragments into a new tour. A k-Opt method uses greedy search within the k-change neighborhood structure. A tour is "k-Opt" if it is locally minimum with respect to the k-change neighborhood structure.

Algorithm LSMC

Input: TSP instance,
iteration bound M,
temperature schedule $temp_i$, $i = 1, \ldots, M$

Output: heuristic tour T_{best}

1. Generate a random tour T_{init};
   $T_1 = Descent(T_{init})$;
   $T_{best} = T_1$;

2. **for** $i = 1$ **to** M
   2.1. $T_i^* = kick_move(T_i)$;
   2.2. $T_i^{**} = Descent(T_i^*)$;
   2.3. $diff = cost(T_i^{**}) - cost(T_i)$;
   if ($diff < 0$) $T_{i+1} = T_i^{**}$;
   else {
   generate a random number $t \in [0, 1)$;
   if ($t < \exp(-diff/temp_i)$);
   $T_{i+1} = T_i^{**}$;
   else
   $T_{i+1} = T_i$;
   }
   2.4. **if** ($cost(T_{best}) > \text{cost}(T_i^{**})$) $T_{best} = T_i^{**}$;

3. **return** T_{best};

Figure 1: The LSMC algorithm

1). Based on experimentally derived intuition, the authors of [Martin, Otto and Felten, 1991] set the temperature used for Boltzmann acceptance to be zero in most cases.[2] Johnson [Johnson, 1990] implicitly also sets the temperature to be uniformly zero. Thus, in both previous studies a new local minimum is generally not accepted unless it strictly improves over the current solution.[3]

It is worth noting that early work of Baum [Baum, 1986a] [Baum, 1986b] proposed an *iterated descent* approach that is essentially similar to the more recent LSMC strategies. However, Baum's implementation suffered from poor choices of the *Descent* and kick move elements: (i) he used 2-Opt and 3-Opt for local optimization, with 2-change kick moves applied until the search was considered to be trapped in a suboptimal basin of attraction; and (ii) he then applied two successive random

[2] In [Martin, Otto and Felten, 1991], the use of non-zero temperature was discussed in the context of the LIN318 example, but no details of the implementation were given.

[3] Martin and Otto [Martin and Otto, 1996] have recently conjectured that for instances of "moderate" size (e.g., the ATT532 instance from TSPLIB) zero-temperature LSMC can be expected to return the global minimum solution, since the LSMC cost surface has at most only a few local minima. That zero-temperature LSMC has very few basins of attraction is also in some sense an implicit assumption of Applegate et al. [Applegate et al., 1995], who use the union of edges in a very small number (10) of LSMC solutions to generate a good bounding solution within a branch-and-bound approach; this method has resulted in several recent "world's records" for optimal solution of large TSP instances.

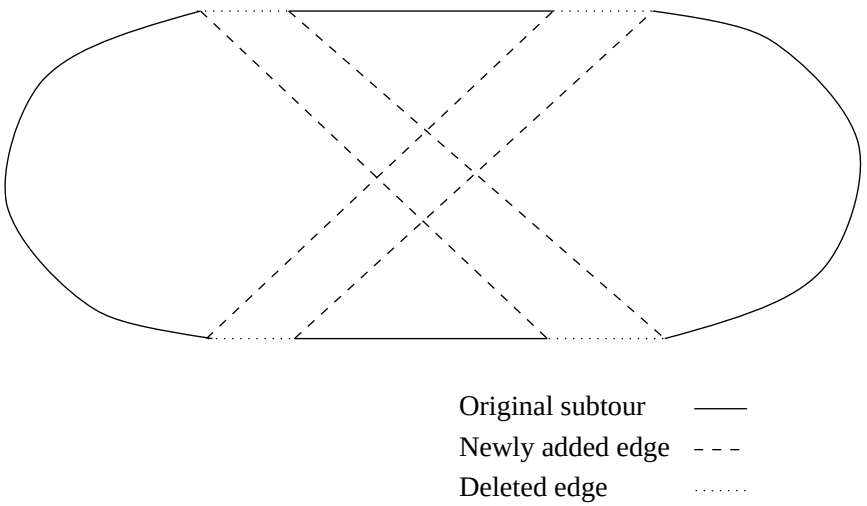

Figure 2: Illustration of the double-bridge 4-change kick move.

2-changes (i.e., a type of 4-change) as a kick move in order to escape the current basin of attraction. Interestingly, Baum's choice of 2-change as the basis of his kick move stemmed from his belief that if a 2- or 3-Opt solution is perturbed by a 2-change, then the next greedy descent will almost always lead to a new local minimum. On the other hand, [Martin, Otto and Felten, 1991] states that the above kick move is generally unable to escape the current basin of attraction (i.e., local optimization will return to the same local minimum); the double-bridge 4-change kick move is partly motivated by this belief. (Our experiments with the LIN318 instance from TSPLIB indicate that a new local optimum is obtained just under 10 percent of the time when 2-change and local optimization are applied to a 2- or 3-Opt solution.)

As a related development in the literature, we note that periodic kick moves of varied size (and strength) are a fundamental theme of the tabu search approach called strategic oscillation [Glover, 1977], which has been applied effectively to diverse combinatorial optimization problems (see, e.g., the survey of [Glover, 1996]). Applications to graph problems often take the form of alternately deleting and then adding (or adding and then deleting) different collections of elements in controlled steps that destroy and then recover feasibility – a pattern that is also achieved by a k-change kick move in the TSP setting. This provides an interesting connection between the strategic oscillation approach and the LSMC approach.

1.2 Scope of the Present Study

In this work, we study the performance of LSMC on randomly-generated symmetric TSP instances[4] using a variety of local optimization heuristics and kick moves. In particular, we examine relationships among (i) the underlying local optimization engine within the LSMC approach, (ii) the "kick

[4]Our instances have distance matrices either (i) corresponding to randomly-generated pointsets in the Euclidean plane, or (ii) corresponding to independent random inter-city distances taken from a uniform distribution.

move" perturbation that is applied between successive local search descents, and (iii) the resulting LSMC solution quality. In Section 2, we show that the traditional "double-bridge" kick move is not necessarily optimum: stronger local optimization engines (e.g., Lin-Kernighan) are best matched with stronger kick moves. In Section 3, we also propose use of a simple adaptive temperature schedule to allow escape from deep basins of attraction; the resulting *hierarchical* LSMC variant outperforms traditional LSMC implementations that use uniformly zero temperatures. Finally, Section 4 studies a population-based LSMC variant wherein multiple solution paths are allowed to cooperate in order to possibly achieve improved solution quality.

Our experiments use 2-Opt, 3-Opt and LK local optimization engines provided by [Boese, 1995]. These codes implement speedups of 2- and 3-Opt which are described in [Bentley, 1992] and reviewed in [Johnson and McGeoch, 1997]. Using a strategy originally due to Lin and Kernighan [Lin and Kernighan, 1973], a *neighbor-list* stores the 25 nearest neighbors for each city; this is implemented via the *k-d* tree [Bentley, 1990] data structure and simplifies finding improving moves or verifying local optimality. Following the terminology of [Johnson, 1990] [Baum, 1986a] [Baum, 1986b], we call the associated LSMC implementations Iterated 2-Opt, Iterated 3-Opt and Iterated LK, respectively.

As testbeds, we use three instances whose optimal tour costs are known. LIN318 and ATT532 are well-known geometric TSP instances used in many other studies, e.g., [Martin, Otto and Felten, 1991] [Martin, Otto and Felten, 1992] [Martin and Otto, 1996] [Johnson, 1990]; the former has 318 city locations and is due to Lin and Kernighan [Lin and Kernighan, 1973], while the latter is derived from the locations of 532 cities in the continental United States. The optimal tour lengths are known to be 42029 (LIN318) and 27686 (ATT532).[5] The third instance is S800, an 800-city random symmetric instance with integer inter-city distances randomly chosen from the interval $[1, 10000]$. The optimal tour length for S800 is known to be 20328 [Applegate, 1995].

Generally, all performance comparisons in this paper are based on the averages of solution costs over 50 trials.[6] The average running times are reported in CPU seconds on an HP-Apollo 9000/735 workstation.

2 Studies of Kick Move Strength

The studies of [Baum, 1986a] [Baum, 1986b] and [Martin, Otto and Felten, 1991] clearly point out the effect of kick move choice on solution quality. Intuitively, the kick move size should be such that (i) it is likely that the search can reach a new basin of attraction, yet (ii) the current level of solution quality is not lost through random perturbation. As noted above, both [Martin, Otto and Felten, 1991] and

[5] City locations are specified by integer coordinates in the Euclidean plane. Inter-city distances are maintained as double-precision reals, and tour costs are rounded to the nearest integer.

[6] The exception is the Iterated LK results for instance S800; running times were such that we are able to report only the average of 2 trials.