AutoOpt: A Methodological Framework of Automatically Designing Metaheuristic Algorithms for Optimization Problems

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Abstract

Metaheuristics are gradient-free and problem-independent search methods. They have gained huge success in solving various optimization problems in academia and industry. Automated metaheuristic algorithm design is a promising alternative to human-made design. This paper proposes a methodological framework, AutoOpt, for automatically designing metaheuristic algorithms for optimization problems. AutoOpt consists of: (1) a bi-level criterion to evaluate the designed algorithms’ performance; (2) a general schema of the decision space from where the algorithms will be designed; (3) a mixed graph- and real number-based representation to represent the designed algorithms; and (4) a model-free method to conduct the design process. AutoOpt benefits academic researchers and practical users struggling to design metaheuristic algorithms for optimization problems. A real-world case study demonstrates AutoOpt’s effectiveness and efficiency.

Keywords: Metaheuristic, Optimization, Evolutionary Algorithm, Automated Design

1. Introduction

Optimization problems are ubiquitous in academia and industry. Metaheuristics are gradient-free and problem-independent search methods. They have gained huge success on solving complex (e.g., non-convex, non-separable, non-differentiable, large-scale, and multi-objective) optimization problems (Eiben and Smith, 2015; Miikkulainen and Forrest, 2021; Liu et al., 2018; Zhao et al., 2021, 2022). Because there is not a specific metaheuristic algorithm that is constantly better than others on all problems (Wolpert and Macready, 1997), human experts are always requested to select, configure, or design algorithms for
different problems. Such human algorithm design has been recognized as laborious, subject to specific assumptions, prone to over-generalization, and biased by human experience and intuition.

Automated metaheuristic algorithm design is an alternative to human design without the above shortcomings. It automatically tailors algorithms for given problems by programming algorithmic operators, composing the operators, and configuring endogenous parameters. The output is existing or unseen algorithm(s) that can efficiently solve the targeted problem. Human intervention is not necessary during the automatic design process. Thus, automated metaheuristic algorithm design makes high-performance algorithms accessible to a much broader range of researchers and practitioners.

Automated metaheuristic algorithm design is functionally different from the terminologies automated algorithm selection (Kerschke et al., 2018), automated algorithm configuration (Huang et al., 2019), and generation hyper-heuristics (Pillay and Qu, 2018). Automated algorithm selection chooses an algorithm from a portfolio, while automated algorithm configuration tunes parameters within a given algorithm. In them, the algorithm’s structure and operators are human-predefined. By contrast, the algorithm’s structure and operators can be automatically designed in automated algorithm design. Generation hyper-heuristic mainly refers to using genetic programming (GP) (Koza, 1994) to generate a heuristic or metaheuristic algorithm (Gendreau et al., 2010). The primary goal is raising the generality of the algorithm (Glover and Kochenberger, 2006; Gendreau et al., 2010; Pillay and Qu, 2021). In comparison, methods and goals of automated algorithm design include but are not limited to GP and generality, respectively.

We summarize the basic workflow of automated metaheuristic algorithm design in Figure 1. According to Figure 1, the objective of automated metaheuristic algorithm design, i.e., the criterion to evaluate the designed algorithm’s performance on the targeted problem, guides the design process to find promising algorithms. The objective can be maximizing the designed algorithm’s solution quality on the targeted problem, minimizing the design’s expected running time, maximizing the area under the empirical cumulative distribution function curve of running times (Ye et al., 2022), or simultaneously pursuing multiple objectives.

The decision space for metaheuristic algorithm design can be constructed in two ways. The first way is using existing algorithmic operators, e.g., genetic crossover and mutation (Eiben et al., 2003), as building blocks to constitute the decision space (Qu et al., 2020; Alfaro-Fernández et al., 2020; Bezerra et al., 2015, 2020; Villalón et al., 2021; Swan et al., 2019). The second way is using basic computational primitives, e.g., +, −, ×, /, add, swap, to construct the decision space (Sim et al., 2015; Nguyen et al., 2021; Tian et al., 2021).

Figure 1: Basic workflow of automated metaheuristic design.
The first way is popular in recent literature (Qu et al., 2020; Alfaro-Fernández et al., 2020; Bezerra et al., 2015, 2020; Villalón et al., 2021; Swan et al., 2019) because it utilizes the ingenuity inspired from nature, e.g., the genetic operator from biological evolution (Eiben et al., 2003), and the particle swarm fly operator from birds’ social behavior (Shi and Eberhart, 1998). The second way searches for algorithmic operators from scratch, which would be non-trivial due to limited computational resources.

For design’s representation, the mixed categorical and numeral representation is normally employed for the decision space constructed by existing algorithmic operators (López-Ibáñez et al., 2016; Hutter et al., 2009). That is, integers or characters index algorithmic operators; continuous or discrete real numbers represent algorithmic parameters. The directed cycle graph has also been employed as an alternative to the mixed representation (Tisdale et al., 2021). The parse tree, linear array, and directed acyclic graph representations from GP (Koza, 1994) are widely adopted for the decision space constructed by computational primitives (Harris et al., 2015). In particular, the linear array and graph representations may require a template to map the designed algorithms from the genotype to phenotype. The Backus Naur Form grammar (Ryan et al., 1998) has acted as a such template (Tavares and Pereira, 2012). The computational primitives have either been defined by users or been collected from the instructions of the Push language (Lones, 2019).

Methods for automated metaheuristic algorithm design (the module within the dotted box in Figure 1) can be divided into model-based and search-based methods. SMAC is one of the representative model-based methods (Hutter et al., 2011; Lindauer et al., 2022). Following the Bayesian optimization paradigm, SMAC uses a random forest surrogate to model the designed algorithm’s performance on the targeted problem. The promising algorithm is predicted and sampled via maximizing the expected improvement acquisition function (Hutter et al., 2011; Lindauer et al., 2022). Search-based methods include irace (López-Ibáñez et al., 2016), ParamILS (Hutter et al., 2009), and GP (Harris et al., 2015) etc. irace is an iterative search version of the F-race method (Birattari and Kacprzyk, 2009). Its key feature is using the racing scheme to eliminate less competitive algorithms in the design selection step (Step 4 in Figure 1). New algorithms will be generated based on the survival algorithms after racing (López-Ibáñez et al., 2016). ParamILS emphasizes on adopting local search to produce new algorithms in the design generation step (Step 2 in Figure 1) (Hutter et al., 2009). The genetic search is employed in the design generation step in the GP-based hyper-heuristic literature (Gendreau et al., 2010).

Most of the above settings, strategies, and methods are originated for algorithm parameter configuration (hyperparameter optimization). Their extensions to metaheuristic algorithm design face challenges, and some of them are not that explicit and straightforward to use. For example, irace offers a powerful tool for the design selection step, ParamILS provides strong insight into the design generation step. Still, almost all works leave the decision space to be user-defined and fail to support design metaheuristics with various structures. A comprehensive methodological framework for automated metaheuristic algorithm design is necessary but still lacking.

To address these challenges, this paper proposes a methodological framework, called AutoOpt, for automatically designing metaheuristic algorithms. AutoOpt is a comprehensive solution to researchers and practitioners who are struggling to design metaheuristic algorithms for optimization problems. In details, it includes 1) a straightforward bi-level
objective function for metaheuristic algorithm design; 2) a general schema for constructing the decision space for metaheuristic design; 3) a mixed graph- and real number-based representation for the bi-level design, which allows designing metaheuristic algorithms with various structures and search behaviors; 4) a method integrated with statistical test and Pareto dominance for selecting promising algorithms generated during the design process. A real-world case study is provided to test AutoOpt’s effectiveness and efficiency.

The remainder of the paper contains: the proposed AutoOpt in Section 2, case study in Section 3, and conclusions in Section 4.

2. AutoOpt

The proposed AutoOpt is a comprehensive methodological framework for automatically designing metaheuristic algorithms for optimization problems. According to the framework, various metaheuristics with flexible structures can be automatically tailored to different problems. AutoOpt follows the workflow in Figure 1 and is detailed below. Its source code is available at https://github.com/qz89/AutoOpt.

2.1 Objective of Metaheuristic Algorithm Design

AutoOpt provides the following objective formulation for automated metaheuristic algorithm design:

\[
\begin{align*}
\text{arg max}_{A_{\text{ops}}, A_{\text{parms}}} & \quad P_{\text{probl}}(A_{\text{ops}}, A_{\text{parms}}), \\
\text{s.t.} & \quad A_{\text{parms}} = \text{arg max}_{A'_{\text{parms}}} P_{\text{probl}}(A_{\text{ops}}, A'_{\text{parms}}),
\end{align*}
\]

where \(A_{\text{ops}}\) and \(A_{\text{parms}}\) are the operators and parameters that consist the designed algorithm \(A\), respectively; \(P_{\text{probl}}(A_{\text{ops}}, A_{\text{parms}})\) measures the performance of \(A\) on the targeted problem \(\text{probl}\). The performance can be measured either by the designed algorithm’s performance obtained within a fixed computational budget or by the designed algorithm’s running time till reaching acceptable performance.

The proposed bi-level formulation decouples the algorithmic operator composition \(A_{\text{ops}}\) and parameter configuration \(A_{\text{parms}}\) into two levels. Such decoupling is straightforward and intuitive for efficient algorithm design because the performance of an algorithmic operator composition subjects to appropriately configuring the endogenous parameters.

2.2 Decision Space for Metaheuristic Algorithm Design

AutoOpt proposes a general schema for constructing the decision space with existing algorithmic operators. The schema is according to the taxonomy in Shi (2018). It is acknowledged that metaheuristics come from human observation and inspiration from biological evolution, swarm cooperation, natural and physical phenomena, etc. From a human innovation point of view, the taxonomy summarizes metaheuristic algorithms’ search behaviors into three categories, i.e., learning, imitating, and exploring (Shi, 2018):

- The learning behaviors learn the converging trend from current individuals and search along with the learned trend. For example, the individual in particle swarm optimization flies toward the direction learned from the global and local best particles (Shi
and Eberhart, 1998); the rand/1 differential evolution searches along the direction obtained from the differential of a pair of randomly selected individuals (Das and Suganthan, 2010).

- The imitating behaviors emulate and inherit information from current individuals. For instance, the Gaussian mutation emulates from a parent subject to a Gaussian disturbance; the one-point crossover inherits genes from a pair of parents (Eiben et al., 2003).

- The exploring behaviors enable the search to jump out from the current area, which provides new possibilities for convergence. The re-initialization during the search process belongs to this category.

Before performing the three categories of search behaviors, metaheuristic algorithms should have the capacity of determining where should be searched from over the solution space of the targeted problem. For example, genetic algorithms use mating selection to select parents; some swarm intelligence algorithms, e.g., particle swarm optimization, search from each individual, respectively. Metaheuristic algorithms should also have the capacity of updating individuals after performing search behaviors. For genetic algorithms, this capacity refers to selecting individuals from parents and offspring; for some swarm intelligence algorithms, this refers to whether accepting or rejecting individual updates.

According to the above taxonomy, we give a schema of the decision space for automated metaheuristic algorithm design in Figure 5 in the Appendix. The proposed schema involves most of the widely-used metaheuristic operators from the evolutionary and swarm algorithm perspective. Other metaheuristic and problem-specific heuristic operators can also been placed into the schema according to the taxonomy.

The proposed schema offers a flexible top-down metaheuristic algorithm design template. The designed algorithms will have at least one search behavior that belongs to learning or imitating categories. The designed algorithms can also have multiple search behaviors that belong to different categories.

### 2.3 Representation of the Designed Algorithms

AutoOpt employs the directed graph to represent metaheuristic algorithm structure, (i.e., algorithmic operator composition $A_{ops}$ in Equation 1). The reason for employing directed graph is that it is flexible to represent algorithms with various structures. In other words, the represented algorithm can involve either one search behavior that belongs to learning or imitating categories (Figure 5) or multiple search behaviors that belong to different categories.

Parameters (i.e., $A_{params}$ in Equation 1) are represented by real numbers. In particular, control variables are associated with representations of search operators’ parameters. These control variables determine the computational resource allocated to each search operator in $A_{ops}$.

An example of the representation is shown in Figure 2. Figure 2(a) represents an algorithm with two search behaviors. One is imitating via one-point crossover and random resetting; another is exploring by reinitialization. In Figure 2(b), the first two entities refer
that 90% and 10% of the individuals will be searched by imitating and exploring, respectively; the third to seventh entities refer the parameters of the binary-tournament selection, one-point crossover, random resetting, reinitialization, and pairwise selection operators, respectively, in which only the random resetting has a parameter of resetting probability that is set to 0.1.

Note that external and problem-specific operators and techniques, e.g., initialization, external archives, constraint-handling, and large-scale solution space decomposition, would be incorporated with algorithms’ phenotype representations for effective problem-solving.

### 2.4 Method for Designing Metaheuristic Algorithms

AutoOpt follows the search-based design scheme due to its flexibility in designing algorithms with different structures and scalability in incorporating various techniques for designing algorithms. We detail the five steps (shown in Figure 1) of AutoOpt’s design method as follows.

#### 2.4.1 Step 1: initializing designs

Designs (i.e., the designed algorithms) can be initialized in two ways. One is cold-start, i.e., randomly sampling algorithms over the decision space. Another is warm-start, i.e., using existing metaheuristic algorithms as the initial designs. AutoOpt supports to simultaneously maintain $N \ (N \geq 1)$ designs during the design process.

#### 2.4.2 Step 2: generating new designs

AutoOpt proposes a simple yet effective local search to generate algorithmic operator compositions (i.e., $A_{ops}$ in the upper level of Equation 1) and employs CMA-ES (Hansen, 2016)
to search for parameters (i.e., \( A'_{\text{params}} \) in the lower level of Equation 1). The reason for using these methods is due to their promising performance observed in our experiment and the recommendation from literature (Fawcett and Hoos, 2016; Hutter et al., 2019). The local search refers to either changing one operator that is randomly selected from the directed graph or changing the directed graph’s structure by adding/deleting one search operator.

2.4.3 Step 3: evaluating designs’ performance

The evaluation can be conducted in two ways. One is exact evaluation, i.e., running the designed algorithms on the targeted problem. Another is approximation, i.e., building a surrogate to approximate designs’ performance on the targeted problem. The former way is accurate and can be used in cases where the targeted problem is computationally cheap and computational resource is adequate. The latter way may not be that accurate but is available for computationally expensive targeted problems.

2.4.4 Step 4: selecting designs

AutoOpt suggests two methods for selecting promising designs from the current ones. The selected designs will be sent back to Step 2 unless the designing process goes into Step 5.

The first method is employing the F-race (Birattari and Kačprzyk, 2009; López-Ibáñez et al., 2016) because of the statistical evidence for algorithm comparison and selection that F-race provides. In this method, F-race is conducted on the current designs and will be terminated once there remain \( N \) designs. These \( N \) designs are the ones being selected.

The F-race is conducted on all targeted problem instances and reveals the overall performance of the designed algorithms across the instances. For targeted problems with heterogeneous instances, one may be interested in designing multiple algorithms that each one specializes in a part of instances and is acceptable for the rest instances. This interest requires performance comparison on each instance rather than across instances. To this end, we propose the second method for selecting designs. In detail, for each pair of designs, the Wilcoxon Sign Test (d Steel and Torrie, 1986) is conducted on the paired designs’ performance on each problem instance, respectively. Then, the paired designs’ Pareto dominance relationship (Deb et al., 2002) in terms of the performance on all problem instances is calculated. Designs that have not been dominated by others are the Pareto nondominate designs. These nondominate designs will be recursively selected until there have been \( N \) selected designs.

For example, suppose there are two problem instances \( p_1, p_2 \) and two designed algorithms \( A_1, A_2 \). \( A_1 \) is better than \( A_2 \) on \( p_1 \), and \( A_1 \) is comparable with \( A_2 \) on \( p_2 \) based on the Wilcoxon Sign Test. According to the Pareto dominance relationship, \( A_1 \) dominates \( A_2 \) because \( A_1 \) is not worse than \( A_2 \) in all instances and is better than \( A_2 \) in at least one instance. As a result, \( A_1 \) is the Pareto nondominate design and is selected.

2.4.5 Step 5: outputting design(s)

AutoOpt can output either the best design for the target problem or multiple (\( \leq N \)) designs to consist of an algorithm portfolio.
3. Case Study

3.1 Problem Description

The problems in the case study come from the supply chain department of a leading biomedical electronics company in China. Material management is one of the main tasks of the supply chain department of this company. This task includes collecting raw materials from upstream suppliers, stacking the materials in warehouses, and picking up and sending materials to the manufacturing department according to requirements. The material stacking problem is challenging due to three reasons: (1) the problem has been proven to be NP-hard (Liu et al., 2019); (2) the materials for producing complex medical electronic products, e.g., computed tomography scanners and blood detection machines, are large-scale and heterogeneous; (3) the materials will be changed according to the changes of manufacturing plans.

The company’s material stacking is decoupled into two problems to reduce difficulty. The first problem (termed as probl$_1$ hereafter) is stacking materials on racks. This is a discrete optimization problem. The decision variables are the materials’ stacking strategies. The objective is to maximize the number of materials that can be stacked on the racks. The second problem (termed as probl$_2$ hereafter) is placing the racks in the warehouse subjecting to some rules, e.g., the materials with high picking up frequencies should be placed near the shipping area. This is a permutation optimization problem. The decision variables are the racks’ placing locations. The objective is to maximize the warehouse’s space usage subjecting to the above rules.

In general, these two problems can be solved in two ways. The first way is relaxing the problems and solving them by integer programming, etc. This way suffers from the inaccuracy occurred by problem relaxation. The second way is using heuristic or metaheuristic algorithms to directly solve the problems. This way cannot provide a mathematical guarantee but is without the inaccuracy from problem relaxation.

The company’s supply chain department staff struggle to solve the problems in either of the two ways due to the lack of optimization problem-solving knowledge and experience. Consequently, the proposed AutoOpt is worth employing to automatically design metaheuristic algorithms for these problems.

3.2 Application of AutoOpt to the Problems

AutoOpt is applied to design a metaheuristic algorithm for probl$_1$ and probl$_2$, respectively. probl$_1$ has a number of 39 instances, i.e., 39 racks need to be stacked. probl$_2$ has 2 instances, i.e., two types of racks in the warehouse will be placed, respectively.

AutoOpt is set as follows. In the objective of metaheuristic algorithm design (i.e., Equation 1), the performance $P_{prob}$ is measured by the designed algorithm’s performance obtained within a fixed computational budget. The budget is set as 5000 fitness evaluations with a population size of 50 for each designed algorithm. The decision space for algorithm design comes from Figure 5, in which search operators marked with # and * are for designing metaheuristics for the discrete problem probl$_1$ and permutation problem probl$_2$, respectively, and updating operators marked with % are for both probl$_1$ and probl$_2$. The cold-start initialization (refers to Section 2.4.1), the exact evaluation (refers to Section 2.4.3), and the
method integrated with statistical test and Pareto dominance (refers to the second method of Section 2.4.4) are employed for the design initialization, evaluation, and selection steps, respectively. $N = 10$ algorithms are maintained in the design process, and the design process iterates 20 times for $prob_1$ and $prob_2$, respectively.

The designed algorithms for $prob_1$ and $prob_2$ are termed as $alg_1$ and $alg_2$, respectively. Their pseudocode are given in Figures 3 and 4, respectively. The performance of $alg_1$ and $alg_2$ are compared with representative metaheuristic algorithms for discrete and permutation problems, respectively, to test AutoOpt’s effectiveness and efficiency. The settings of the comparison are as follows. $alg_1$ is compared with a discrete genetic algorithm (GA). The discrete GA consists of the traverse, one-point crossover, random resetting, and greedy selection operators. The mutation probability is set to $1/D$, where $D$ is the dimension of the solution space of the targeted problem instance. $alg_2$ is compared with a permutation GA consisting of the traverse, order (two-point) crossover, insert mutation, and greedy selection operators. The performance of the comparing algorithms is obtained by setting the population size as 50, the maximum number of fitness evaluations as 5000, and 30 runs on each problem instance, respectively.

The performance of the comparing algorithms are provided in Tables 1 and 2, respectively. It can be seen that $alg_1$ obtains better results than the discrete GA in most of the instances of $prob_1$, and $alg_2$ is overall comparable with the permutation GA on $prob_2$. These results present preliminary evidence of AutoOpt’s efficiency in designing metaheuristic algorithms for optimization problems. Further comparisons with other metaheuristics and exact methods (i.e., these with problem relaxation and math programming) are desirable, which will be done soon.
Table 1: Average fitness values among 30 runs of the algorithm designed by AutoOpt, i.e., \( alg_1 \), and the discrete GA on each instance of \( probl_1 \). Better results are bold.

| Instance No. | AutoOpt | GA | Instance No. | AutoOpt | GA | Instance No. | AutoOpt | GA |
|--------------|---------|----|--------------|---------|----|--------------|---------|----|
| 1            | 230400  | 230400 | 16          | 32864776.6 | 44557736.1 | 31          | 22110746 | 39423746 |
| 2            | 7309931.35 | 13249931.4 | 17          | 2779055.5 | 8477055.5 | 32          | 51287626 | 74579626 |
| 3            | 7470001 | 19674001 | 18          | 926673.08 | 2066673.08 | 33          | 41530783.8 | 53441287.8 |
| 4            | 2254588.25 | 2578588.25 | 19          | 23027240.8 | 28516840.8 | 34          | 70462672.5 | 12251867.3 |
| 5            | 1789625.63 | 3982952.63 | 20          | 29266831.4 | 45754314.6 | 35          | 35778023.6 | 57715044.6 |
| 6            | 24373250.6 | 48085250.6 | 21          | 44747782.6 | 56697826.6 | 36          | 20256661.6 | 44340216.6 |
| 7            | 24014628.7 | 44456504.7 | 22          | 26634342.9 | 36104276.1 | 37          | 28194853 | 50599733 |
| 8            | 32294761 | 48661886 | 23          | 90669771.3 | 94098513.3 | 38          | 22526095.4 | 33855245.9 |
| 9            | 15933757.3 | 26877957.3 | 24          | 5442447945 | 652244625 | 39          | 13347982 | 25787982 |
| 10           | 737807.23 | 16901807.2 | 25          | 10010316.1 | 15458232.1 |            |            |     |
| 11           | 112414768 | 108983626 | 26          | 1438253 | 13089253 |            |            |     |
| 12           | 32298710.5 | 59424965.5 | 27          | 5066022 | 81260222.38 |            |            |     |
| 13           | 2144215 | 3512115 | 28          | 6146231.3 | 95238641.1 |            |            |     |
| 14           | 37433536.9 | 414142978.9 | 29          | 94026106 | 65279814.2 |            |            |     |
| 15           | 34133016.5 | 50347128.5 | 30          | 79097852.2 | 106641760 |            |            |     |

Table 2: Average fitness values among 30 runs of the algorithm designed by AutoOpt, i.e., \( alg_2 \), and the permutation GA on each instance of \( probl_2 \). Better results are bold.

| Instance No. | AutoOpt | GA |
|--------------|---------|----|
| 1            | 1920    | 1910 |
| 2            | 2500    | 2760 |

4. Conclusions

This paper proposes a comprehensive methodological framework AutoOpt for designing metaheuristic algorithms for optimization problems. In particular, the proposed framework provides a bi-level objective formulation, a general schema of decision space, a mixed graph- and real number-based representation, and a selection method with statistical test and Pareto dominance for designing metaheuristic algorithms. Overall, AutoOpt provides a comprehensive solution for researchers and practitioners who are struggling to design metaheuristic algorithms for their optimization problems.

Automated metaheuristic algorithm design is an emerging topic in which there are many open issues. For example, accelerating the design process, incorporating prior knowledge into the design process, online metaheuristic design, incremental metaheuristic design, and explanation of metaheuristic design.

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Appendix

The proposed schema of decision space for automated metaheuristic algorithm design is depicted in Figure 5.

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Figure 5: Schema of the decision space from the evolutionary and swarm algorithm perspective for automated metaheuristic design. Traverse refers to search from each individual, respectively. Local resetting is the local search version of random resetting, in which the reset is conducted over the neighbor area around the current individual. Accept update means always accepting individual updates. For example, the new location of each particle will always be accepted in particle swarm optimization; the offspring always replace the parents in the $(\mu, \lambda)$ genetic algorithm. The three categories of search operators marked with # and * are for discrete and permutation problems, respectively, while these without marks are for continuous problems. Updating operators marked with % and $ are for single- and multi-objective problems, respectively. The decision space of operators’ inner parameters depends on the bounds of parameter values. Details of the operators and inner parameters are enclosed in the readme file of the AutoOpt source code.