# Bit-Vector Algorithms for Binary Constraint Satisfaction and Subgraph Isomorphism

JULIAN R. ULLMANN, King's College London

A solution to a binary constraint satisfaction problem is a set of discrete values, one in each of a given set of domains, subject to constraints that allow only prescribed pairs of values in specified pairs of domains. Solutions are sought by backtrack search interleaved with a process that removes from domains those values that are currently inconsistent with provisional choices already made in the course of search. For each value in a given domain, a bit-vector shows which values in another domain are or are not permitted in a solution. Bit-vector representation of constraints allows bit-parallel, therefore fast, operations for editing domains during search. This article revises and updates bit-vector algorithms published in the 1970's, and introduces focus search, which is a new bit-vector algorithm relying more on search and less on domain-editing than previous algorithms. Focus search is competitive within a limited family of constraint satisfaction problems.

Determination of subgraph isomorphism is a specialized binary constraint satisfaction problem for which bit-vector algorithms have been widely used since the 1980s, particularly for matching molecular structures. This article very substantially updates the author's 1976 subgraph isomorphism algorithm, and reports experimental results with random and real-life data.

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## 1. INTRODUCTION

Determination of subgraph isomorphism, that is, finding whether a given graph is a subgraph of a further given graph, is an example of a binary constraint satisfaction problem [Mackworth 1977], in which we seek one or more combinations of discrete values of a given set of $V = \{V_1, \ldots, V_i, \ldots, V_n\}$ of $n$ variables so as to satisfy

*Unary constraints*. Values of a variable $V_i$ must belong to a given finite domain, $D_i$, of discrete values.

*Binary constraints*. Values of variables $V_i$ are constrained to satisfy a given set $C$ of binary predicates $P_{ij}$, such that if $V_i$ takes on the value $u$, then $V_j$ can take on the value $v$ if and only if $P_{ij}(u, v)$.

Author's address: J. Ullmann, Department of Informatics, King's College London, Strand, London WC2R 2LS, UK; email: jrullmann@acm.org.

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A solution, $z = (z_1, \ldots, z_i, \ldots, z_n)$, is an $n$-tuple such that

—$z_i \in D_i$ for all $1 \leq i \leq n$, and
—If there is a constraint between variables $V_i$ and $V_j$, then $P_{ij}(z_i, z_j)$.

We seek solutions by using enhanced backtrack search [Golomb and Baumert 1965], which instantiates successive variables. *Instantiate* means assign a trial value. After instantiating some variables, the search process checks whether constraints that should now be satisfied are actually satisfied. If they are satisfied, then a further variable is instantiated; otherwise, the most recently assigned value is changed. When all values have been tried, the search backtracks to reinstantiate a previously instantiated variable, and so on.

After a set, $W$, of variables have been instantiated, let $Z_W$ be the set of solutions such that in each solution in $Z_W$, each variable in $W$ has its instantiated value. If there is no solution in $Z_W$ that includes a value $v$ of a variable $V_i$, then the set $Z_W$ of solutions is unchanged if $v$ is removed from domain $D_i$. *Domain reduction* means removal of values that cannot be included in a solution. Domain reduction is intended to reduce the number of combinations explored during backtrack search.

Although this constraint satisfaction problem is NP-Complete [Cook 1971], algorithms that interleave domain reduction with backtrack search have a substantial community of practical users, for example [Boutselakis et al. 2003; Artymiuk et al. 2005; Klukas et al. 2005; Durand et al. 2006]. Practical effectiveness inevitably depends upon implementational detail, which in turn depends upon the representation of constraints. To avoid re-evaluation of predicates, all evaluation can be done just once, prior to commencement of backtrack search, which now works with a stored representation of constraints. For example, we can store a tabular representation of $P_{ij}$, which is the set of all ordered pairs $(u, v)$ of values such that $P_{ij}(u, v)$ is **true** [Lecoutre 2009]. A different tabular representation of $P_{ij}$ is the set of all ordered pairs $(u, v)$ of values such that $P_{ij}(u, v)$ is **false**.

This article is primarily concerned with representation of a predicate $P_{ij}$ by a one-dimensional array $M^i_j$ of sets such that $M^i_j[u] = \{v | P_{ij}(u, v)\}$. Thus, $P_{ij}(u, v) \equiv v \in M^i_j[u]$. As is very well known, a set can be represented by a bit-vector that has one bit corresponding to each possible member. A bit is "1" if and only if the corresponding member is present in the set. We represent sets by bit-vectors, on which an ordinary CPU can perform bit-parallel intersection and union operations, thus gaining speed.

Bit-vector representation was used in the 1970s for seeking subgraph isomorphism [Ullmann 1976] and also for general binary constraint satisfaction [McGregor 1979]. During the next thirty years, bit-vector isomorphism algorithms were widely employed in practice, particularly in molecule matching applications [Willett et al. 1998]. During the same period the artificial intelligence community developed constraint satisfaction algorithms working directly with predicates, or instead with tabular representations thereof [Bessière 2006], but usually not with bit-vector representation. Perhaps this was because bit-vector representation provides no complexity-theoretic benefit. However, from the viewpoint of practical performance, authoritative experimentation [Lecoutre and Vion 2008] suggests strongly that, for binary constraints, bit-vector implementation has not been surpassed in the artificial intelligence literature.

In order to benefit from bit-parallelism, domain reduction procedures in Section 3 of this article represent domains, as well as binary constraints, by bit-vectors. When the search backtracks, domains must be restored to an appropriate previous state. Bit-vectors representing domains can be saved/restored by push/popping a stack, incurring

considerable cost in time and memory. Section 4 introduces focus search, which is a new algorithm that avoids save/restore. In Section 5, the use of surrogate values can decrease the length of bit-vectors, thus reducing memory requirements and increasing the speed of search.

Section 6 applies the technology of previous sections in the determination of subgraph isomorphism, which is a specialized constraint satisfaction problem wherein

—No two values in a solution $z$ may be the same.
—Specialized unary constraints may greatly reduce the work done by a search process.
—Bit-vector memory requirements are reduced when the same constraint predicate $P_{ij}$ applies to more than one pair $(i, j)$ of variables.

Subgraph isomorphism has well-established practical relevance in chemoinformatics [Leach and Gillet 2003; Brown 2009].

Before reporting experiments with isomorphism, Section 7 reports experiments with randomly generated constraint satisfaction problems and also with radio frequency assignment problems, emphasizing that isomorphism is not the only important practical application for binary constraint satisfaction algorithms.

Domain reduction in Sections 3 and 4 is based on the well-known idea of support, which is revised in Section 2.

## 2. SUPPORT

### 2.1. Full Support

After instantiating a set $W$ of variables, we need to identify values that cannot now belong to any solution. Identification is based on simple inference, for which we use the following well-established definitions. A *graph* is a set of vertices and a set of edges that are pairs of these vertices. The *degree* of a vertex is the number of edges that include it. Two vertices are said to be *adjacent* if they belong to the same edge.

Corresponding to a binary constraint satisfaction problem we define a constraint graph, wherein vertices correspond to variables and edges correspond to pairs of variables that are subject to binary constraints. Two variables are adjacent if and only if they are the subject to the same binary constraint. We define $A_i$ to be the set of variables that are adjacent to the variable $V_i$. Moreover, $C_{ij}$ is the constraint between variable $V_i$ and a variable $V_j \in A_i$.

If there is a constraint between $V_i$ and $V_j$, then in any solution $z$, we must have $P_{ij}(z_i, z_j)$. Therefore, a value $u$ in the domain $D_i$ of $V_i$ cannot belong to any solution unless there is a value $v \in D_j$ such that $P_{ij}(u, v)$. A value $v \in D_j$ such that $P_{ij}(u, v)$ is said to *support* $u \in V_i$ [Bessière 2006; Naanaa 2009]. A value $u \in D_i$ that is supported by at least one value in domain $D_j$ is said to be supported in constraint $C_{ij}$. A value $u \in D_i$ that is not supported in constraint $C_{ij}$ cannot belong to any solution. Going further, a value $u \in D_i$ is said to be fully supported if and only if it is supported in every constraint $C_{ij}$ such that $V_j \in A_i$. A value $u \in D_i$ that is not fully supported cannot belong to any solution and can, therefore, be removed from domain $D_i$.

The set of solutions remains unchanged if values that are not fully supported are removed from domains. Removal of values from domains may remove support for values in other domains, so there may be propagation of removal from domains as in [Ullmann 1965]. At convergence, which is the situation where there is no further removal because every value in every domain is fully supported, the constraint structure is said to be arc consistent [Mackworth 1977; Bessière 2006].

After each instantiation, we invoke a domain reduction procedure that attempts to simplify subsequent search by removing unsupported values from domains. Some

versions of this procedure propagate removal until convergence,[1] others do not. If domain reduction empties any domain when a set $W$ of variables have been instantiated, then there is no solution that includes these instantiations. In this case, nothing can be achieved by instantiating further variables; instead the backtrack search reinstantiates a variable in $W$.

When domain $D_i$ is inferentially reduced to a single value, we have implied instantiation of the variable $V_i$, whereas instantiation by the search process is elective [Lynce and Marques-Silva 2003]. Suppose that immediately after elective or implied instantiation of $V_i$, domain reduction continues until convergence. Consider a constraint $C_{ij}$ such that domain $D_j$ is multivalued at convergence. At this time, we can be sure that every value in $D_j$ is supported by the single value of $V_i$. Equally surely, the single value of $V_i$ is supported by every value in $D_j$. While further variables are instantiated, the single value of $V_i$ remains supported in constraint $C_{ij}$ so long as $D_j$ is not empty. If any domain is empty the search does not proceed. Therefore, we do not need to check whether the value of $V_i$ is supported in constraint $C_{ij}$ after further instantiation. This is true for every constraint $C_{ik}$ such that $V_k \in A_i$, so if domain $D_i$ is single-valued at the time of convergence, then nothing is achieved by checking whether the value in $D_i$ is supported after further instantiations. Lecoutre [2008] has emphasized that it is unnecessary to check whether electively instantiated values are supported, and this idea appears also at Line 5 in Figure 2 in Bessière et al [2008]. We now go further by observing that it is also unnecessary to check whether implied instantiated values are supported. This means that after an elective instantiation we only need to check whether values in multivalued domains are supported. Here, multivalued means multivalued at the time of convergence in a previous invocation of a domain reduction procedure, since when there has been neither backtrack nor reinstantiation.

If, to improve efficiency, we apply domain reduction only to multivalued domains, then the first application requires attention. If domain $D_i$ is single-valued initially, before the first application of domain reduction, then we cannot then be sure that its value is fully supported. We deal with this simply by removing all unsupported values from domains during preprocessing prior to commencement of search, as in Section 3.3.

### 2.2. Bit-Vector Representation of Support Sets

We represent predicate $P_{ij}$ by a one-dimensional array, $M_j^i$, of sets initialized so that $M_j^i[u] = \{v | P_{ij}(u, v)\}$. In this $M_j^i$ notation, the superscript identifies the variable whose values select elements of the one-dimensional array; the subscript identifies the other variable involved in the constraint. Each set $M_j^i[u]$ is represented by a bit-vector.

The bit-vector $M_j^i[u]$ can be regarded as a row of a bit-matrix $M_j^i$. If the rows of this matrix are packed into words to allow bit-parallel operations, the columns are not. The row $M_j^i[u]$ allows bit-parallel operations on the set of all values of $V_j$ that can be supported in constraint $C_{ij}$ by value $u \in D_i$. We also require bit-parallel operations on the set of all values of $V_i$ that can be supported in constraint $C_{ij}$ by value $u \in D_j$. For this purpose, we employ a second bit-matrix $M_i^j$, initialized so that $M_i^j[u] = \{v | P_{ij}(v, u)\}$, with rows selected by values of the superscript variable. For this second bit-matrix, $P_{ij}(v, u) \equiv (v \in M_i^j[u])$. Representing $P_{ij}$ both by $M_j^i$ and also by its transpose $M_i^j$ obviously requires twice as much memory as just one of these representations. All

[1]Maintaining arc consistency, abbreviated to MAC, is a widely used name for a family of constraint satisfaction backtrack algorithms, which, after each instantiation, propagate removal until arc consistency is achieved, as in Ullmann [1976, 1977], McGregor [1979], and Sabin and Freuder [1994].

```
procedure search;
input:  Dsets, which is an array [1..n] of bit-vectors such that Dsets[i] represents domain D_i
          initialized according to unary constraints; also
          initialized bit-matrices (to be referenced by the domain reduction procedure);
output: Line 13 records all solutions.
begin
1   initialize domains, stacks, instantiation sequence and weights;
2   choose(i, terminal); (* Select variable V_i to be instantiated next and
              also return terminal = (all domains are single-valued). *)
3   initialize search for untried values in domain D_i;
4   repeat
5     if there are any untried values in domain D_i then
6       push(i, Dsets); (* This saves a copy of i and also of Dsets *)
7       v := next untried value in domain D_i;
8       D_i := {v}; (* Instantiating Variable V_i to value v *)
9       reduce(i, Dsets, consistent); (* Domain reduction procedure *)
10      if consistent then (* No domain is empty, so proceed *)
11        choose(i, terminal); (* Select variable V_i to be instantiated and
                also return terminal = (all domains are single-valued). *)
12        if terminal then (* All domains are single-valued *)
13          output this solution;
14          pop(i, Dsets) (* Restore before trying another value *)
15        else initialize search for untried values in newly chosen D_i;
16          (* The next iteration will instantiate the newly chosen V_i *)
17        end if;
18      else pop(i, Dsets) (* Restore before trying another value of the same variable *)
19      end if;
20    else (* Backtrack to the previous variable *)
21      if stack is not empty then pop(i, Dsets) (* to restore these *) end if
22    end if;
23  until stack is empty;
end search;
```

Fig. 1. Outline of a backtrack search algorithm that finds all solutions to an instance of the constraint satisfaction problem.

bit-matrices have the same dimensions such that their rows are bit-vectors in which the number of bits is always the maximum cardinality, $\delta$, of any domain.

Constraints are symmetric if all predicates in a given binary constraint satisfaction problem are such that $P_{ij}(u, v) = P_{ij}(v, u)$; otherwise, constraints are asymmetric. For symmetric constraints, we have $M_j^i[u] = \{v|P_{ij}(u, v)\}$ and $M_i^j[u] = \{v|P_{ij}(v, u)\}$, so $M_j^i = M_i^j$ and we only need one bit-matrix to represent each predicate. As will be explained in Section 6.1, subgraph isomorphism with unordered graphs is an example of a symmetric constraint satisfaction problem: Adjacency matrices of unordered graphs are symmetric.

## 3. BASIC BIT-VECTOR DOMAIN REDUCTION ALGORITHMS

### 3.1. A Backtrack Search Algorithm

The backtrack algorithm[2] outlined in Figure 1 employs dynamic variable ordering [Lecoutre 2009, Section 9.1.1], which means that the instantiation sequence may vary during the search. Procedure *choose* uses the *dom/wdeg* heuristic

[2]This algorithm generally tries many successive values for each variable. Binary branching, which is an alternative strategy, tries just one value before selecting another variable [Lecoutre 2009, Page 362].

[Boussemart et al. 2004] employing weights $\{w_{ij}\}$ to select the next variable, $V_i$, for elective instantiation.[3] Procedure *choose* is shown in Appendix Section A.2.

To process values in a domain in turn serially, as at Line 7 in Figure 1, we can search for successive 1's in the domain's bit-vector. Instead, to save time, we can avoid visiting 0's in bit-vectors by representing each domain by an array, as well as by a bit-vector, so we have duplicate representation. During the search, the duplicate representation must be saved and restored[4] together with the bit-vector representation. Appendix Section B gives details.

Save/restore via a stack, as in Figure 1, is *pop-stack* domain restoration. The stack must be able to accommodate $n$ copies of an array of $n$ bit-vectors. When the number, $n$, of variables is large (e.g., $n > 1{,}000$), and when the maximum number, $\delta$, of values in a domain is also large, the amount of memory required for $\delta n^2$ bits may require attention. Instead of pushing the entire array, *Dsets*, of domain bit-vectors onto a stack, we only need to push bit-vectors that have changed, since they were last pushed. These are easily identified, but at the cost of slowing the search.

If we use array (as well as bit-vector) representation of domains, we do not need a stack of arrays of domain bit-vectors. Array representation readily shows which values should be restored to domains, so individual bits can be changed from "0" to "1" accordingly. Appendix Section B.1 gives further details of this method of restoration, which we call *incremental* restoration.[5] Incremental restoration reduces memory requirements but is usually slower than pop-stack restoration that uses microprogrammed iteration to move a bock of data within memory.

### 3.2. A Bit-Vector Direct Reduction Procedure

This section introduces the first of three versions of the domain reduction procedure *reduce* that is called at Line 9 in Figure 1. The set of values in $D_j$ that support $u \in D_i$ is $\{v | P_{ij}(u, v)\} \cap D_j$. This set is represented by the bit-vector $M_j^i[u]{*}Dsets[j]$, where "*" denotes bit-wise **and** and $Dsets[j]$ is a bit-vector representing $D_j$. In bit-vector *direct* reduction [Ullmann 1976; Lecoutre and Vion 2008], a value $u$ is removed[6] from domain $D_i$ as soon as procedure *reduce* finds that $M_j^i[u]{*}Dsets[j] = 0$, where 0 is a bit-vector that represents the empty set.

Following McGregor [1979], the direct reduction procedure in Figure 2 uses a queue[7] of ordinals that identify variables; we think of this as being a queue of variables. If a domain $D_i$ is reduced by removal of at least one value, then $i$ is inserted into the queue

[3]This heuristic associates a score with each variable that is a candidate for elective instantiation because its domain is not already single-valued [Lecoutre 2009, Section 9.3.1] For the variable $V_i$, this score is $|D_i|/(\sum_{j \in \breve{A}_i} w_{ij})$, where $|D_i|$ is the current cardinality of domain $D_i$, and $\breve{A}_i = \{V_k | (V_k \text{ is adjacent to } V_i) \wedge (|D_k| > 1)\}$ and $w_{ij}$ is a weight associated with the unordered pair $\{V_i, V_j\}$ as follows. Initialization assigns $w_{ij} := 1$. During the search, the weight $w_{ij}$ is increased by one when no value in $D_i$ is supported by $D_j$ or when no value in $D_j$ is supported by $D_i$. Procedure *choose* selects the variable for which the score is minimal.

[4]Lecoutre and Vion [2008] employ linked list duplicate representation. Array representation, with swapping as in Briggs and Torczon [1993], is somewhat faster because values can be restored to domains in constant time without being processed serially one by one.

[5]In other terminology [Schulte 1999], incremental restoration is an example of *trailing* and pop-stack restoration is an example of *copying*.

[6]If $I$ is a bit-vector that represents $D_i$, and if $U$ is a bit-vector that represents $\{u\}$, and if $u \in D_i$, then $u$ can be removed from $I$ by $I := exclusiveOr(I, U)$.

[7]Represented by an array of ordinals and also by a bit-vector to allow rapid checks for set membership. Our experiments employ a simple first-in first-out queue because bit-vector reduction is so fast that the overheads of managing a priority queue [Wallace and Freuder 1992; Boussemart et al. 2004] appear to outweigh the benefit.

```
procedure reduce(in h: integer; in out Dsets: array of bit-vectors; out consistent: boolean);
input:  h identifies the variable that has just been instantiated;
        Bit matrices are accessed via global variables;
input and output: Dsets is an array of bit-vectors representing domains;
output: consistent = (no domain is empty);
begin
1   initialize queue to be empty; insert h into queue;
2   repeat
3     j:= variable removed from queue;
4     for each i such that V_i is adjacent to V_j and D_i is multivalued do
            (* multivalued means multivalued at the time of invocation of this procedure *)
5       changed:= false;
6       for u:= each value that is currently in D_i do
7         if M_j^i[u] * Dsets[j] = 0 then (* There is no support in D_j for u in D_i *)
8           remove u from D_i; changed:= true;
9           if D_i is empty then w_ij:= w_ij + 1; consistent:= false; return end if;
10        end if
11      end for;
12      if changed and (i ∉ queue) then
          insert i into queue (* i will subsequently be a j that is removed from the queue *)
        end if;
13    end for;
14  until queue is empty; (* The procedure has reached convergence *)
15  consistent:= true;
end reduce;
```

Fig. 2. An introductory outline of a bit-vector direct reduction (BVDR) implementation of procedure *reduce*.

to enable a subsequent iteration to check whether any value in an adjacent domain is no longer fully supported and should, therefore, be removed.

Appendix Section A.1 explains how, for each variable, we maintain a linked list of adjacent variables that have multivalued domains at the time of invocation of this procedure. **For each** at Line 4 in Figure 2 is implemented efficiently by traversing this list. Within this list for $V_j$, the record for the adjacent variable $V_i$ includes a pointer to the bit-matrix $M_j^i$. This is how the procedure accesses bit-matrices.

At Line 6, we can find values currently in $D_i$ by searching for 1's in $Dsets[i]$. Instead, to avoid visiting 0's in bit-vectors, we can use duplicate (bit-vector and array) representation of domains, as in Appendix Section B.1, although this does not always make the search faster.

### 3.3. A Bit-Vector Cumulative Reduction Procedure

With direct reduction, the innermost loop (Lines 6 through 11 in Figure 2) is the part of the entire search-and-reduction algorithm that is executed most frequently. McGregor [1979] used cumulative reduction[8] to simplify and optimize the innermost loop. Cumulative reduction is so called because it accumulates supported values (in a bit-vector $B$ in Figure 3) instead of eliminating unsupported values immediately. Lines 4 and 6 in Figure 3 can be implemented in the same way as Lines 4 and 6 in Figure 2.

It is sometimes helpful to call procedure *reduce* between Lines 1 and 2, as well as at Line 9, in Figure 1. Domain reduction before commencement of search is an example

[8]Cumulative reduction has also been employed in Ullmann [1977], Lecoutre [2008], and Cheng and Yap [2010].

```
procedure reduce(in h: integer; in out Dsets: array of bit-vectors; out consistent: boolean);
input:  h identifies the variable that has just been instantiated;
        Bit matrices are accessed via global variables;
input and output: Dsets is an array of bit-vectors representing domains;
output: consistent = (no domain is empty);
begin
1   initialize queue to be empty; insert h into queue;
2   repeat
3     j:= variable removed from queue;
4     for each i such that V_i is adjacent to V_j and D_i is multivalued do
5       B:= 0; (* A bit-vector wherein all bits are 0. This represents an empty set. *)
6       for v := each value that is currently in D_j do
          (* M_i^j[v] is the set of possible values of variable V_i supported by value v in D_j *)
7         B:= B + M_i^j[v]    (* '+' denotes bitwise inclusive-or, implementing set union *)
8       end for;
9       B := Dsets[i] * B;    (* B := {u ∈ D_i | u is supported by value(s) in D_j} *)
10      if Dsets[i] ≠ B then (* D_i has been reduced *)
11        if B = 0 then w_ij:= w_ij + 1; consistent:= false; return end if
12        Dsets[i]:= B; (* reducing domain D_i *)
13        if (i ∉ queue) then insert i into queue end if;
14      end if;
15    end for;
16  until queue is empty; (* at convergence *)
17  consistent:= true;
end reduce
```

Fig. 3. An introductory outline of a bit-vector cumulative reduction (BVCR) implementation of procedure *reduce*.

of *preprocessing*. When used for preprocessing, the bit-vector cumulative reduction (BVCR) procedure is modified so that

—All variables are put in the queue initially, and
—*All* adjacent variables are processed, whether or not their domains are initially multivalued, and
—There is no provision for restoring eliminated values, because these are permanently eliminated from domains.

When any domain is empty there can be no solution, so the search does not proceed. Note also that if a domain is single-valued before commencement of search, we cannot be sure that its single value is fully supported. In this case, the direct and cumulative domain reduction procedures work correctly only after preprocessing.

### 3.4. A Bit-Vector Forward-Checking Procedure

The domain reduction procedures in Sections 3.2 and 3.3 usually reduce a domain most when they process it for the first time. If procedures are curtailed so that no domain is reduced more than once, this obviously takes less time but achieves less reduction than when reduction continues until convergence. McGregor [1979, Figure 5] introduced a simple curtailed reduction procedure that was given the name *Forward checking* by Haralick and Elliott [1980]. Forward checking[9] deserves attention because, in some circumstances, constraint satisfaction problems can be solved more quickly and simply by using this instead of the procedures in Sections 3.2 and 3.3. With forward checking, the number of elective instantiations is much higher, but much less domain reduction work is done after each instantiation.

[9]Forward checking is an embodiment of *preclusion* [Golomb and Baumert 1965].

```
procedure forwardCheck(in j, v : integer; in out Dsets: array of bit-vectors;
                       out consistent: boolean);
input: j identifies the variable that has just been instantiated;
       v is the value that has been assigned to j by elective instantiation;
       Bit matrices are accessed via global variables;
input and output: Dsets is an array of bit-vectors representing domains;
output: consistent = (no domain is empty);
begin
1  for each variable V_i adjacent to V_j that has not been electively instantiated do
2    Dsets[i]:= Dsets[i] * M_i^j[v];  (* D_i := D_i ∩ {u|u is supported by v ∈ D_j}.
     This assignment eliminates from D_i every value that is not supported by v ∈ D_j *)
3    if Dsets[i] = 0 then w_ij := w_ij + 1; consistent:= false; return end if;
4  end for
5  consistent:= true;
end forwardCheck;
```

Fig. 4. An introductory outline of a forward-checking domain reduction procedure.

The forward-checking procedure in Figure 4 is called instead of procedure *reduce* at Line 9 in Figure 1. Line 2 in Figure 4 is executed for adjacent variable $V_i$ even if domain reduction has already reduced $D_i$ to a single value. This is because the single value in $D_i$ may not be supported by the value $v$ of $V_j$. At the time of invocation of the forward-checking procedure, every value in the domain of every variable that has not yet been electively instantiated is certainly supported by the value of every adjacent variable that was electively instantiated previously. But a value in the domain of a variable that was not electively instantiated previously may not be supported by any value in the domain of an adjacent variable that was not electively instantiated previously: Forward checking does not check this.

With forward checking, we use a version of procedure *choose* that may return $i$ such that $V_i$ has already been instantiated by implication. This is because procedure *forwardCheck*, when called after elective instantiation of an implied-instantiated variable, may remove values from further domains, thus speeding up the search [Ullmann 2007]. Appendix Section A.2 includes this version of procedure *choose*, and explains how Line 1 in Figure 4 avoids visiting adjacent variables that have not been electively instantiated.

If the forward-checking version of procedure *choose* finds that all domains are single-valued, then it returns *terminal* = **true**, but there is no guarantee that values of variables that have not been electively instantiated are fully supported. In other words, it is possible that the single values now in domains may not constitute a solution because there may be constraints that are not satisfied. To deal with this, the search could continue until all except one of the variables have been electively instantiated, but this would be unnecessarily inefficient. Instead, after the forward-checking version of procedure *choose* returns *terminal* = **true**, the search process calls a procedure *allSatisfied*, which explicitly checks that all binary constraints are satisfied. A combination of values, one in each domain, is accepted as a solution only if all constraints are satisfied.

## 4. FOCUS SEARCH

### 4.1. The Static Instantiation Sequence in Focus Search

When domain reduction is interleaved with backtrack search, a domain may be restored before any benefit has been obtained from its reduction. In this respect, domain

```
 1: AA------------------
 2: B-B-----------------
 3: -C-C----------------
 4: ---DD---------------
 5: E---EE--------------
 6: --F-FFF-------------
 7: --G-G--G------------
 8: ------H-H-----------
 9: -------III----------
10: J-------J-J---------
11: K-------K--K--------
12: --------L---L-------
13: ---------M--MM------
14: ------------NNN-----
15: ------------OO-O----
16: ----P--------P--P---
17: ----Q-----------QQ--
18: --R-------------R-R-
19: ------------S-----SS-
20: ---T----------T-----T
```

Fig. 5. An example in which columns correspond to successive variables in the static instantiation sequence $0, 1, \ldots, n-1$. There is one row corresponding to each variable except the first. In the row corresponding to $V_h$, the *location* of the rightmost letter identifies $V_h$. Locations of other letters in this row identify preceding variables in $Y_h$ that are adjacent to $V_h$.

reduction processes are inevitably inefficient. Focus search is so called because it focuses reduction primarily on a small number of uninstantiated domains that may soon be instantiated electively. Focus search does not entirely avoid fruitless reduction operations, but it does avoid saving and restoring the results of these operations during the search. Like forward checking, focus search does not apply domain reduction iteratively until convergence; instead, again like forward checking, focus search relies on a very large number of invocations of a simple domain reduction procedure. Compared with bit-vector cumulative reduction, forward checking performs a very much larger number of elective instantiations; therefore, the total cost of saving and restoring domains during the search is very much higher. It is important that focus search entirely avoids save/restore during the search.

For forward checking, another consequence of the large number of instantiations is that a large total amount of time is spent selecting successive variables for instantiation. Focus search avoids spending this time by working instead with a static instantiation sequence that is fixed before commencement of search and remains unchanged thereafter.

Section 2.2 explained that the procedures in Section 3 require duplicate representation of asymmetric constraint predicates: A predicate $P_{ij}$ is represented both by $M_j^i$ and also by the transpose $M_i^j$. Because of its static instantiation sequence, focus search does not require this duplicate representation. For example, if $V_7$ precedes $V_3$ in the instantiation sequence, then $M_3^7[v]$ will at some time be required but $M_7^3[v]$ will never be required because $V_3$ will never be instantiated before $V_7$.

In the static instantiation sequence for focus search, let $Y_i$ be the set of variables that precede and include the variable $V_i$. The variable $V_{i+1}$ is chosen so as to maximize[10] the number of variables in $Y_i$ that are adjacent to $V_{i+1}$. An example in Figure 5 indicates

[10]This differs from the maximum cardinality algorithm of Tarjan and Yannakakis [1984] only in that ties are not broken arbitrarily.

```
procedure reduce(i: integer; out consistent: boolean);
input:  i identifies the variable that has just been instantiated;
        Bit matrices are accessed via global variables;
output: Dsets is an array of bit-vectors representing domains;
        consistent = (no domain is empty);
begin
1   for each j such that (V_i ∈ pastAdj(V_j)) ∧ (i ≠ λ(j)) do
        (* for each j such that i is an adjacent predecessor, but not the last, of j do *)
2     jD := ∩_{V_h ∈ prec(i,j)} M_j^h[f(h)]; (* jD := {v|v is supported by the
        instantiated value of every variable in Y_i that is adjacent to V_j} *)
3     if jD = 0 then consistent:= false; return end if;
4   end for;
5   for each j such that i = λ(j) do (* for each j such that i is the
        last adjacent predecessor of j do *)
6     jD := ∩_{V_h ∈ pastAdj(V_j)} M_j^h[f(h)]; (* jD := {v|v is supported by the
        instantiated value of every variable in Y_i that is adjacent to V_j} *)
7     if jD = 0 then consistent:= false; return end if;
8     Dsets[j] := jD;
9   end for;
10  consistent:= true;
end reduce;
```

Fig. 6. Focus search procedure *reduce*. Here, $jD$ is a bit-vector of the same type as $Dsets[j]$.

the variables in $Y_i$ to which a variable $V_{i+1}$ is adjacent. In many cases, more than one variable not in $Y_i$ is adjacent to the largest number of variables in $Y_i$: Such ties are broken by a heuristic that favors the variable for which the sum of the branches of its adjacent variables is maximal. Here, *branches* of a variable $V_i$ means the sum of the degrees of the variables to which $V_i$ is adjacent.

### 4.2. Focused Domain Reduction

Like the algorithms in Section 3, focus search is a backtrack search algorithm that calls a domain reduction procedure *reduce* immediately after each elective instantiation. Each of the algorithms in Section 3 achieves both of the following effects in the same way.

(1) Reduction of the number of values to which a variable $V_i$ will be instantiated, thus reducing the number of elective instantiations.
(2) Avoidance of parts of the search space that do not include any solution. If after instantiation of $V_i$ the domain of any not-yet-instantiated variable contains no value that is fully supported, then the search proceeds no further until at least one variable has been reinstantiated.

In focus search, these two effects are achieved in different ways, both involving $pastAdj(V_i)$, which is the set of variables in $Y_i$ that are adjacent to $V_i$. $V_i$ is not included in $pastAdj(V_i)$. Within $pastAdj(V_i)$, $\lambda(i)$ is the last; therefore, closest to $V_i$, in the static sequence. In Figure 6, which outlines procedure *reduce* for focus search, $f(h)$ is the current instantiated value of the variable $V_h$.

To achieve the first effect, focus search waits until all variables in $pastAdj(V_j)$ have been instantiated and then, at Line 8 in Figure 6, makes $D_j$ be the set of all values of $V_j$ that are supported by values of variables in $pastAdj(V_j)$. The intention is that domain reduction is focused on the single domain $D_j$ from which values of $V_j$ will next be selected for instantiation. Actually domain reduction is not so exactly focused because $V_i$ may possibly be the last variable in $pastAdj(V_j)$ for more than one $j$, as can be seen

in Figure 5. For example, if $V_{\lambda(j)} = V_{\lambda(j+3)}$, then, immediately after instantiation of $V_{\lambda(j)}$, Lines 5 through 9 in Figure 6

—remove from $D_j$ all values that are not supported by values of variables in $pastAdj(V_j)$ and
—remove from $D_{j+3}$ all values that are not supported by values of variables in $pastAdj(V_{j+3})$

If any domain is now empty, procedure *reduce* returns *consistent* = **false**.

If, between the times of instantiation of $V_{\lambda(j)}$ and $V_j$, there is backtrack such that a variable $V_k$ after $V_{\lambda(j)}$ and before $V_j$ in the static sequence is reinstantiated, then $D_j$ is not affected because, by definition of $V_{\lambda(j)}$, $V_k$ is not adjacent to $V_j$. If backtrack is such that $V_{\lambda(j)}$ is reinstantiated then Lines 5 through 9 in Figure 6 recompute $D_j$. For these reasons, focus search does not save/restore $D_j$.

Lines 1 through 4 in Figure 6 achieve the second of the two effects mentioned in the first paragraph of this section,[11] after instantiation of the variable $V_i$. In Line 1, the condition $(i \neq \lambda(j))$ prevents duplication of work that will be done at Lines 5 through 9. At Line 2, $prec(i, j) = pastAdj(V_j) \cap Y_i$, which means that $prec(i, j)$ is the set of instantiated adjacent predecessors of $V_j$. At Line 2, focus search does not store the result bit-vector $jD$ and, therefore, does not need to save/restore it. As well as avoiding save/restore, an advantage of not saving $jD$ is that when this consists of hundreds of bits, copying it to memory takes appreciable time. A disadvantage is that, during subsequent invocations, Line 6 in Figure 6 in some cases recomputes intersections that were computed at Line 2 and could have been stored during previous invocations of procedure *reduce*.

The focus search procedure *reduce* assumes that initialization has ensured that every value in $M_j^h[v]$ is also in the initial $D_j$, which is specified as part of the original formulation of the problem. This is why $D_j^{initial}$ is not included in the intersection at Lines 2 and 6 in Figure 6.

### 4.3. The Search Procedure in Focus Search

Like the previous backtrack search procedure in Figure 1, focus search instantiates a variable $V_i$ to successive values that are currently in domain $D_i$. Focus search employs a linked list of values that could possibly be in $D_i$, and refers to $Dsets[i]$ to check whether each successive value is currently in $D_i$. For $V_i$, the list could simply contain all values in $D_i^{initial}$, that is, the initial contents of $D_i$ specified as part of the problem formulation. However, the following development improves efficiency.

For each variable $V_i$, except the first variable in the static instantiation sequence, we arbitrarily select just one variable, $V_h$, say, from the set $pastAdj(V_i)$. The selected variable $V_h$ is the *selector* for $V_i$. For each possible value, $u$, of the selector $V_h$, we initialize $seLists[i, u]$ to be a linked list representation of the set $M_i^h[u] \cap D_i^{initial}$. As before, $M_i^h[u]$ represents the set of possible values of $V_i$ that are supported by the value $u$ of $V_h$. Thus, $seLists[i, u]$ represents the set of values in $D_i$ supported by the value $u$ in $D_h$. At Line 10 in Figure 7, $selector[i] \uparrow = u$ such that $u$ is the currently instantiated value of $V_h$, where $V_h$ is the selector for $V_i$. What this achieves is that Line 5 only checks values that could be in $D_i$ when $V_h = u$.

When $i = lastVar$ at Line 11, each value in $Dsets[lastVar]$ is certainly included in a solution, so there is no need to execute the loop at Line 3 through 24. Instead, Line 12 calls procedure *lastInstantiation*, which is

[11] Focus search works correctly, but not so fast, if Lines 1 through 4 are omitted.

```
procedure focusearch;
input:  Dsets which is an array [1..n] of bit-vectors such that Dsets[i] represents domain D_i;
        initialized bit-matrices (to be referenced by the domain reduction procedure);
output: All solutions.
begin
1   initialize the instantiation sequence; initialize lists outlined in Section 4.4;
    initialize array successor so that successor[i] identifies the successor of V_i in the
    instantiation sequence; initialize array predecessor so that
    predecessor[i] identifies the predecessor of V_i in the instantiation sequence;
    predecessor[firstVar]:= nil; (* firstVar is the first variable in the instantiation sequence *)
2   i := firstVar; next[i]:= initialDlist; valuePtr:= initialDlist; (* points to list of
              possible values of firstVar *)
3   loop
4     if valuePtr ≠ nil then (* there is an untried value of V_i *)
5       if valuePtr↑.value in Dsets[i] then (* this value is in D_i *)
6         v:= valuePtr↑.value; (* instantiate V_i to this value *) valueAt[i] ↑:= v;
              (* so procedure reduce can access v without dereferencing an array element *)
7         reduce(i, consistent); (* attempt domain reduction *)
8         if consistent then (* search can proceed *)
9           next[i]:= valuePtr↑.nextValue; (* pointing to next possible value of V_i *)
10          i:= successor[i]; valuePtr:= seLists[i, selector[i] ↑];
              (* valuePtr now points to the first possible value of the new V_i *)
11          if i = lastVar then (* all variables except V_lastVar have been instantiated;
                lastVar is the last in the instantiation sequence *)
12            lastInstantiation(valuePtr, Dsets[i]); (* this instantiates V_i to each in
              turn of its available values without calling procedure reduce  *)
13            i:= predecessor[i]; (* backtrack *)
14            valuePtr:= next[i]; (* points to the next untried value of this V_i *)
15          end if;
16        else valuePtr:= valuePtr↑.nextValue; (* points to the next untried value *)
17        end if
18      else valuePtr:= valuePtr↑.nextValue (* points to the next untried value *)
19      end if;
20    else (* backtrack *)
21      i:= predecessor[i];
22      if i = nil then exit (* end of search *)
        else valuePtr:= next[i]; (* points to next untried value of V_i after backtrack *)
        end if;
23    end if;
24  end loop;
25  conclude;
end
```

Fig. 7. The search procedure in focus search.

```
while valuePtr ≠ nil do
  if valuePtr↑.value in Dsets[i] then output solution end if;
  valuePtr:= valuePtr↑.nextValue
end while;
```

This includes each value currently in *Dsets*[*lastVar*] in a separate solution. If only one solution is required, we amend this procedure to **return** after the first solution is found.

### 4.4. List Structures for Focus Search

Focus search needs to identify $V_{\lambda(j)}$ as the last variable in *pastAdj*($V_j$) at the time of instantiation of $V_{\lambda(j)}$. This would be impossible if dynamic variable ordering were

applied. Another reason for using a purely static instantiation sequence is that we are able to construct lists, prior to commencement of search, that enable procedure *reduce* to find all $h$ such that $V_h \in pastAdj(V_j)$ without searching through any $h$ such that $V_h \notin pastAdj(V_j)$. Prior to commencement of search, focus search also builds further list structures, as follows.

For each variable, $V_j$, there is a linked list comprising one record for each variable, $V_{j_k}$, in $pastAdj(V_j)$. The information in each such record is

—An ordinal, $k$, that identifies the variable $V_{j_k}$,
—A pointer, which is the same as $valueAt[k]$, pointing to the current value $f(j_k)$ of $V_{j_k}$,
—A pointer to the bit-matrix that should be used at Lines 2 and 6 in Figure 6, and
—A pointer to the next record in $pastAdj(V_j)$.

The intersection at Line 6 in Figure 6 is implemented efficiently by traversing this list.

For each variable, $V_i$, focus search also has a linked list in which each record points to a $pastAdj(V_j)$ list, as in the previous paragraph, such that $i = \lambda(j)$. This list, which may be empty, enables procedure *reduce* to find quickly all $j$ such that $i = \lambda(j)$. This is how **for each** is implemented at Line 5 in Figure 6.

For each variable $V_i$, focus search has yet another linked list, for use at Line 1 in Figure 6. In the list for $V_i$ there is one record for each $V_j$ such that $V_i \in pastAdj(j)$ and $i \neq \lambda(j)$. Each such record points to a linked list of members of $prec(i, j)$. A list of members of $prec(i, j)$ does not require additional memory because physically it is a sublist of the $pastAdj(V_j)$ list. This is achieved by sorting the records in each $pastAdj(V_j)$ list so that they contain variables in the reverse of the instantiation sequence. Thus, the first variable in the $pastAdj(V_j)$ list is $V_{\lambda(j)}$; the last variable in this list is, within $pastAdj(V_j)$, the earliest variable in the instantiation sequence. The list for $prec(i, j)$, which is used for computing the intersection at Line 2 in Figure 6, is implemented by a pointer to the record for $V_i$ in the $pastAdj(V_j)$ list.

As mentioned in Section 4.3, for each variable $V_i$ and for just one of variable, $V_h$, that precedes $V_i$ in the instantiation sequence, focus search has a separate linked list of records for each value, $u$, in $D_h^{initial}$. This is a linked list representation of the set $M_i^h[u]$. The total memory required for these lists depends on the average cardinality of $\{v|P_{ij}(v, u)\}$.

All of the lists used by focus search are constructed before the start of the search and are not changed thereafter. Of course, these lists contribute to the total memory requirement for focus search. However, focus search does not maintain for each variable $V_i$ a linked list of currently multivalued variables adjacent to $V_i$. Focus search does not have memory requirements, such as a stack of arrays of domains, associated with save/restore. Moreover, focus search does not require duplicate bit-matrix representation of asymmetric predicates.

### 4.5. The Search Tree

For analytical purposes, we can construct a search tree in which nodes correspond to elective instantiations. A node's descendent branches represent values successively assigned to that node by instantiation. If forward checking (FC) and focus search solve the same problem, both using the same static instantiation sequence, with values in domains remaining in the same static sorted order, their search trees are identical.

To see this, assume inductively that the search trees of both algorithms are identical up to the time immediately before instantiation of $V_i$. We need to show that forward checking (FC) and focus search will successively instantiate $V_i$ to the same set of values and that the truth-value of *consistent* will be the same for each such instantiation.

After instantiating a variable $V_h$ a value $u$, FC removes from the domains of all uninstantiated adjacent variables all values that are not supported by $V_h = u$. When this has been done for $V_h$ and, previously, for each of its predecessors, the domain of an uninstantiated variable $V_j$ is

$$D_j^h = \{v \in D_j^{initial} | v \text{ is supported by the values of all variables in } pastAdj(j) \cap Y_h\}.$$

Whereas FC instantiates a variable $V_j$ to each value in $D_j^{j-1}$, focus search instantiates $V_j$ to each value in $D_j^{\lambda(j)}$, which is the set represented by $Dsets(j)$ at Line 8 in Figure 6. By definition, no predecessor variable later than $\lambda(j)$ is adjacent to $V_j$. Therefore, $pastAdj(j) \cap Y_h = pastAdj(j) \cap Y_{\lambda(j)}$, whence FC and focus search instantiate $V_j$ to the same set of values.

After domain reduction following instantiation of a variable $V_i$, let $D_j^i$ be the domain of an uninstantiated variable $V_j$. FC returns *consistent* = **false** if and only if any $D_j^i$ is empty. At Line 3 in Figure 6, focus search returns *consistent* = **false** if and only if any $D_j^i$ is empty, where $i \neq \lambda(j)$. At Line 7, focus search returns *consistent* = **false** if and only if any $D_j^i$ is empty, where $i = \lambda(j)$. Thus, FC and focus search return the same truth-value of *consistent*.

When FC is not confined to the static instantiation sequence of focus search, the FC search tree is usually substantially smaller, but for each elective instantiation, FC does more work than focus search. Appendix C explains that focus search is not merely a binary-constraint version of partition search, although both of these algorithms do belong to the same family.

## 5. SURROGATE VALUES

Long bit-vectors are physically implemented as arrays of single-word bit-vectors. Operations such as bitwise **and** and **or** require word-by-word processing, taking time that depends on the number of words. For this reason, and, more obviously, to reduce memory requirements, it is desirable to minimize the number of words by minimizing the total length of each bit-vector.

In the initial formulation of a constraint satisfaction problem, the discrete values given in each domain are the *data* values. A domain $D_i$ may contain $\delta_i$ data values within a range $lowerBound \ldots upperBound$ such that $upperBound - lowerBound$ is very much greater than $\delta_i$. Examples are given in Section 7.2.

When $upperBound - lowerBound \gg \delta_i$, it may be worthwhile to work with *surrogate values* in the range $0..\delta_i - 1$ instead of the original data values. The advantage is that we now have shorter bit-vectors that comprise $\delta$ bits, where $\delta$ is the maximum, over all domains, of $\delta_i$. Memory requirements are reduced; bit-vector operations are faster.

We use a two-dimensional array $S$ to convert data values to surrogate values. The bounds of the first subscript are $1..numberOfDomains$; the bounds of the second subscript are $0..\delta - 1$. Array element $S[i, u]$ contains a data value, $x$, that is unique within domain $D_i$. The subscript $u$ is the surrogate value that we use instead of the data value $x$. For each domain, $D_i$, the array $S$ implements a function $S_i$ such that $x \equiv S_i(u)$. The surrogate value $u$ uniquely represents the data value $x$ in this domain.

We use the symbol $D_i$ to represent a domain given as part of the initial formulation of the constraint satisfaction problem; for notational simplicity, we use the same symbol $D_i$ to represent the domain comprising surrogate values that represent data values in the original domain $D_i$. We solve a constraint satisfaction problem by working with domains

containing these surrogate values, and applying surrogate predicates $P^s_{ij}$ defined by

$$P^s_{ij}(u, v) \equiv P_{ij}(S_i(u), S_j(v)),$$

where $P_{ij}(x, y)$ is a predicate given in the original formulation of the problem. A surrogate solution, $z^s$, consists of exactly one surrogate value in each domain, satisfying $P^s_{ij}(z^s_i, z^s_j)$ for all $i, j$ such that there is a constraint between $V_i$ and $V_j$. Let $z$ be a set of data values, one in each domain, such that the value in domain $D_i$ is $S_i(z^s_i)$. By construction, $z$ satisfies $P_{ij}(S_i(z^s_i), S_j(z^s_j))$ for all $i, j$ such that there is a constraint between $V_i$ and $V_j$, so $z$ is a solution to the original problem. A solution to the original problem can be obtained from a surrogate solution $z^s$ simply by replacing each value $z^s_i$ in $z^s$ by $S[i, z^s_i]$.

Predicates in frequency assignment problems in Section 7.2 are symmetric, but the derived surrogate predicates are not. Consider, for example, the simple predicate $P_{ij}(x, y) = |x - y| > 8$, where $|x - y|$ denotes the absolute value of $x - y$. If

$$\begin{array}{ll} S_i(1) = -5 & S_j(1) = -3 \\ S_i(2) = 6 & S_j(2) = 2 \end{array}$$

then

$$\begin{aligned} P^s_{ij}(1, 2) &= |S_i(1) - S_j(2)| > 8 = \textbf{false} \\ P^s_{ij}(2, 1) &= |S_i(2) - S_j(1)| > 8 = \textbf{true} \end{aligned}$$

Because surrogate predicates are asymmetric, the memory requirement for surrogate bit-matrices is $2e\delta^2$ bits, where $e$ is the number of binary constraints. With original data values instead of surrogates, and with symmetric predicates, the memory requirement for bit-matrices is $e\Delta^2$ bits, where $\Delta = upperBound - lowerBound + 1$.

## 6. SUBGRAPH ISOMORPHISM

### 6.1. Constraint Satisfaction Problem Formulation

A graph $G = (V, E)$ consists of a set $V = \{V_1, \ldots, V_n\}$ of vertices and a set $E$ of edges, which are unordered pairs of vertices in $V$. There is a subgraph isomorphism between a graph $G^\alpha = (V^\alpha, E^\alpha)$ and a graph $G^\beta = (V^\beta, E^\beta)$ if and only if $G^\alpha$ is isomorphic to a subgraph of $G^\beta$. A *subgraph isomorphism* is a function $I : V^\alpha \to V^\beta$ such that $(V^\alpha_i, V^\alpha_j) \in E^\alpha \Rightarrow (I(V^\alpha_i), I(V^\alpha_j)) \in E^\beta$ and $(i \neq j) \Rightarrow (I(V^\alpha_i) \neq I(V^\alpha_j))$. Thus, a subgraph isomorphism is an injective function from $V^\alpha$ to $V^\beta$ that preserves adjacency. In almost all of the many practical applications of subgraph isomorphism mentioned by Messmer and Bunke [2000], attributes are associated with the vertices and edges of $G_\alpha$ and $G_\beta$; the attributes of corresponding vertices and edges are required to match. However, to review the basic business of subgraph isomorphism, we start by considering graphs that are not labeled with attributes and are not directed.

From the viewpoint of constraint satisfaction, variables identify vertices of the graph $G^\alpha$. Possible values for these variables are identifiers of vertices of the graph $G^\beta$. A constraint satisfaction problem is to assign to each vertex in $V^\alpha$, a value that identifies a vertex in $V^\beta$, subject to

*Unary constraints.* The set $D_i$ of allowed values of a variable $V^\alpha_i$ identify vertices of $G^\beta$ such that $u \in D_i$ if and only if there is no known a priori reason why vertex $V^\beta_u$ in $G_\beta$ cannot correspond to vertex $V^\alpha_i$ of $G_\alpha$ in a subgraph isomorphism. For example, $u \notin D_i$ if the degree of vertex $V^\beta_u$ of $G_\beta$ is less than the degree of vertex $V^\alpha_i$ of $G_\alpha$.

*Binary constraints.* For each $(i, j) \in E^\alpha$, we have a predicate $P_{ij}(u, v) = (u, v) \in E^\beta$.

*AllDifferent constraint.* Every variable in $V^\alpha$ has a value that differs from the value of every other variable in $V^\alpha$.

It is immediately clear that a subgraph isomorphism assigns values to variables so as to satisfy all of these constraints [McGregor 1979]. It is equally easy to see that every solution to this constraint satisfaction problem is a subgraph isomorphism.

For general binary constraints, Section 1 introduced $M_j^i[u] = \{v|P_{ij}(u, v)\}$. For subgraph isomorphism, this becomes $M_j^i[u] = \{v|(u, v) \in E^\beta\}$. Thus, $M_j^i[u]$ is a bit-vector that represents the set of all vertices of $G_\beta$ that are adjacent to $V_u^\beta$. In other words, $M_j^i$ is exactly the same thing as the adjacency matrix of the graph $G_\beta$.

Section 2.2 said that constraints are symmetric if and only if $P_{ij}(u, v) = P_{ij}(v, u)$. When graphs are not directed, $V_u^\beta$ is adjacent to $V_v^\beta$ if and only if $V_v^\beta$ is adjacent to $V_u^\beta$; in this case, for subgraph isomorphism, $M_j^i$ is symmetric. Every edge in $E^\alpha$ has the same constraint predicate, which is represented by the same symmetric matrix, which is the adjacency matrix of $G_\beta$. When graphs are not directed and not labeled, the overall total number of matrices required is one. In this context, we denote this single matrix by $M$.

### 6.2. Invariant Domain Reduction

Domain reduction in Section 3 is *propagational* in the sense that removal of values from one domain may lead to removal of values from further domains, and so on. For isomorphism, *invariant* domain reduction is another important practical means of removing values from domains. A *vertex invariant* is a vertex property such that two vertices can correspond in a graph isomorphism only if their vertex invariants are identical. A simple example is the degree of a vertex [Corneil and Kirkpatrick 1980]; another example is a tuple whose components are the degrees of adjacent vertices sorted into decreasing order. Yet another [Fowler et al. 1983] is a tuple whose components are distance degrees, sorted into sequence of increasing distance. The *distance* between two vertices is the number of edges in the shortest path between these two vertices. The *distance-k-degree* of vertex $V_i$ is the number of vertices at distance $k$ from $V_i$. McKay [2009] lists many further vertex invariants. Invariant domain reduction is achieved by

—Determining vertex invariants of graph $G^\alpha$ in isolation from graph $G^\beta$.
—Determining vertex invariants of graph $G^\beta$ in isolation from graph $G^\alpha$.
—Evaluating, for each pair of vertices $V_i^\alpha$ and $V_u^\beta$, a predicate whose arguments are the vertex invariants of $V_i^\alpha$ and $V_u^\beta$, and removing $u$ from domain $D_i$ if this predicate returns **false**.

For graph isomorphism, but not for subgraph isomorphism, this predicate returns **true** if and only if the vertex invariants of $V_i^\alpha$ and $V_u^\beta$ are identical. For graph isomorphism, it is useful to partition the set of vertices of a graph into subsets such that no two vertices within the same subset have different vertex invariants. This is *vertex partitioning*, which is fundamental to the success of Nauty [McKay 2009].

For subgraph isomorphism, we need to specify allowed differences between the vertex invariants of $V_i^\alpha$ and $V_u^\beta$. This specification can be formulated as a predicate that returns **false** if the vertex invariants of $V_i^\alpha$ and $V_u^\beta$ are such that $V_u^\beta$ cannot correspond to $V_i^\alpha$ in a subgraph isomorphism. A simple example is a predicate that returns **false** if and only if the degree of $V_i^\alpha$ exceeds the degree of $V_u^\beta$. Section 6.4.2 provides further examples.

The essential difference between propagational and invariant domain reduction is that propagational domain reduction removes $u$ from domain $D_i$ if $u$ is not fully supported by current domains of variables that are adjacent to $V_i$. Invariant domain reduction *ignores* domains of variables that are adjacent to $V_i$. From the viewpoint of the constraint satisfaction literature, invariant domain reduction simply removes values that do not satisfy unary constraints. This is not mandatory: The propagational bit-vector cumulative reduction (BVCR) algorithm works correctly if no unary constraints are applied and instead each domain is initialized to be $\{v|V_v^\beta \in V^\beta\}$. However, by applying unary constraints derived from vertex invariants we may reduce the time taken by subsequent preprocessing and search, without changing the outcome of the search.

Although the VF2 algorithm subgraph isomorphism algorithm [Cordella et al. 2004] is not propagational, it uses vertex-matching properties that vary during the search. Cordella et al. have formulated this algorithm for the case where graphs are directed. For simplicity, we now consider related domain-reduction rules for undirected graphs, using the following definition of *past* and *future* degree

—$pastDegreeOf(V_i^\alpha)$ = cardinality of $\{V_j^\alpha | V_j^\alpha$ is adjacent to $V_i^\alpha$ and the variable that corresponds to $V_j^\alpha$ is now electively instantiated$\}$.
—$futureDegreeOf(V_i^\alpha)$ = cardinality of $\{V_j^\alpha | V_j^\alpha$ is adjacent to $V_i^\alpha$ and the variable that corresponds to $V_j^\alpha$ is not currently instantiated$\}$.

We define $pastDegreeOf(V_u^\beta)$ and $futureDegreeOf(V_u^\beta)$ similarly, except that $V_u^\beta$ is here said to be instantiated electively if and only if there exists $V_i^\alpha$ that is currently instantiated electively such that $D_i = \{u\}$. The BVCR algorithm could possibly be developed to apply the following extra domain reduction rule: Include $u$ in $D_i$ only if

$$(pastDegreeOf(V_i^\alpha) \leq pastDegreeOf(V_u^\beta)) \text{ and}$$
$$(futureDegreeOf(V_i^\alpha) \leq futureDegreeOf(V_u^\beta)).$$

Suppose that, for BVCR, domains are initialized so that $u \in D_i$ only if $degreeOf(V_i^\alpha) \leq degreeOf(V_u^\beta)$. Consider a value $u$ that survives in any domain $D_i$ immediately after the BVCR domain reduction procedure has returned *consistent* = **true**. Every instantiated vertex $V_j^\alpha$ that is adjacent to $V_i^\alpha$ has a single-valued domain at this time. If $D_j = \{v\}$, then, since *consistent* = **true**, $V_v^\beta$ is adjacent to $V_u^\beta$. Therefore, $pastDegreeOf(V_i^\alpha) = pastDegreeOf(V_u^\beta)$. Initialization has ensured that $degreeOf(V_i^\alpha) \leq degreeOf(V_u^\beta)$, so $futureDegreeOf(V_i^\alpha) \leq futureDegreeOf(V_u^\beta)$. Therefore, the proposed extra domain reduction rule has no effect because it is necessarily satisfied when the BVCR domain reduction procedure returns *consistent* = **true**.

Taking a step closer to VF2 [Cordella et al. 2004], the BVCR algorithm could possibly be developed to apply the additional domain reduction rule: include $u$ in $D_i$ only if

$$CardinalityOf(\{V_v^\beta \text{ adjacent to } V_u^\beta | \, pastDegreeOf(V_v^\beta) > 0\})$$
is not less than
$$CardinalityOf(\{V_j^\alpha \text{ adjacent to } V_i^\alpha | \, pastDegreeOf(V_j^\alpha) > 0\})$$

Immediately after the BVCR domain reduction procedure has returned *consistent* = **true**, then, as in the previous paragraph, for any value $u$ in any domain $D_i$, $pastDegreeOf(V_i^\alpha) = pastDegreeOf(V_u^\beta)$. At this time, $u \in D_i$ only if for each $V_j^\alpha$ adjacent to $V_i^\alpha$ there exists $v \in D_j$ such that $V_v^\beta$ is adjacent to $V_u^\beta$. Since $pastDegreeOf(V_v^\beta) =$

*pastDegreeOf*$(V_j^\alpha)$ the proposed additional domain reduction rule is necessarily satisfied and so has no effect within BVCR, although such rules may be valuable within VF2.

### 6.3. Bit-Vector Algorithms with the AllDifferent Constraint

*6.3.1. Cumulative and Direct Reduction.* With direct and with cumulative reduction, it is helpful to propagate the *allDifferent* constraint, as follows. When a domain becomes single-valued due to elective or implied instantiation, this single value should be deleted from all currently multivalued domains. If a further domain thereby becomes single-valued, then this single value should also be deleted from all currently multivalued domains, and so on.

We modify the direct reduction procedure, Figure 2, so that if the domain of a variable removed from the queue is single-valued, this value is removed from all other domains that include it. If this makes any domain be empty, then the procedure returns *consistent* = **false**. Otherwise, if a value is removed from domain $D_h$, then $h$ is inserted into the queue. With direct reduction, each iteration of the outermost loop deals with single-valued domains before attempting domain reduction using binary constraints.

When a variable, $j$, is removed from the queue in the isomorphism version of the cumulative reduction procedure, the cardinality of the $D_j$ is generally not known. Values in $D_j$ are counted while using binary constraints to reduce domains of adjacent variables. Afterwards, if $D_j$ is found to be single-valued, then this value is removed from all other domains that include it, and we proceed as in the previous paragraph. In this version of the cumulative reduction procedure, each iteration of the outermost loop attempts domain reduction using binary constraints before dealing with single-valued domains.[12] For direct and cumulative reduction, Section B.3 gives procedural details using duplicate (i.e., bit-vector plus array) representation of domains.

When seeking isomorphism, we use a cumulative reduction preprocessing routine that starts by putting successively at the head of queue all the variables whose domains are initially single-valued, and also by putting all other variables successively at the tail of the queue, as in Section 3.3. This preprocessing routine applies and propagates the *allDifferent* constraint as in the previous paragraph.

*6.3.2. The* AllDifferent *Constraint in Forward Checking.* Procedure *forwardCheck* is called just after a variable has been instantiated to a value $v$. As well as applying binary constraints, the isomorphism version of this procedure enforces the *allDifferent* constraint simply by removing the value $v$ from all other domains that include it. If this empties any domain, then the procedure returns *consistent* = **false**. Procedure *forwardCheck* does not propagate the *allDifferent* constraint.

Section 3.4 noted that when the forward-checking version of procedure *choose* finds that all domains are single-valued, we cannot be sure that all constraints are satisfied. With isomorphism forward checking, we also cannot be sure that the *allDifferent* constraint is satisfied. We, therefore, use a version of the constraint-checking procedure *allSatisfied*, which also checks that all values are different. When procedure *choose* returns *terminal* = **true**, we have a solution only if procedure *allSatisfied* finds explicitly that all constraints, including the *allDifferent* constraint, are satisfied.

[12]In effect there is a constraint $P_{i,j}(u, v) = (u \neq v)$ between every pair of variables, but this is not enforced in the same way as other binary constraints. Instead, we wait until $D_i$ or $D_j$ is single-valued. If $D_i = \{u\}$, we remove $u$ from $D_j$. If $D_j = \{v\}$, we remove $v$ from $D_i$. At convergence of direct or cumulative reduction, all such constraints are satisfied.

*6.3.3. The* AllDifferent *Constraint in Focus Search.* For subgraph isomorphism, focus search is always preceded by preprocessing,[13] which initially imposes the *allDifferent* constraint. Preprocessing initializes *allowed* to be the set of all $i$ such that $D_i$ is multivalued at completion of preprocessing. This set is represented by a bit-vector of the type that represents a domain. In effect, Line 5 in Figure 7 is changed to

**if** valuePtr↑.value **in** (Dsets[$i$] $*$ *allowed*) **then**

so a variable can only be instantiated to allowed values. When a variable $V_j$ is instantiated to a value $v$, this value is removed from the set *allowed*, to prevent instantiation of other variables to the value $v$. Before $V_j$ is reinstantiated, and also before the search backtracks to a preceding variable, this value $v$ is restored to the set *allowed*. The focus search procedure *reduce* is modified so that, in effect, $jD := jD \cap allowed$ is inserted between Lines 2 and 3, and also between Lines 6 and 7, in Figure 6. Thus, $jD$ cannot contain values belonging to domains that are already single-valued. Like forward checking, focus search does not propagate the *allDifferent* constraint.

For focus search, the static instantiation sequence is determined after completion of preprocessing. Variables whose domains are single-valued after preprocessing and before commencement of search are put at the beginning of the instantiation sequence and are not visited by the search because they do not require reinstantiation. This arrangement is essential because during the search

**if** valuePtr↑.value **in** (Dsets[$i$] $*$ *allowed*) **then**

prevents instantiation of domains that are already single-valued.

When one or more variables are excluded from the search because their domains are initially single-valued, the following situation arises. An excluded variable may be $V_{\lambda(i)}$ for a variable $V_i$ whose domain is initially multivalued, so *Dsets*[$i$] will not be properly determined by the focus search procedure *reduce*. In this case, we assign to *Dsets*[$i$] the bit-vector that represents domain $D_i$ at the time of return from the preprocessing procedure.

### 6.4. The LocalI *allDifferent* Constraint

*6.4.1. Bipartite Matching.* Let $A_i^\alpha$ be the set of all vertices adjacent to vertex $V_i^\alpha$ in $G^\alpha$. Similarly, let $A_u^\beta$ be the set of all vertices adjacent to $V_u^\beta$ in $G^\beta$. If an isomorphism, $I$, exists such that $I(V_i^\alpha) = V_u^\beta$, then there exists an injective function $L : A_i^\alpha \to A_u^\beta$ such that

—For all $V_j^\alpha \in A_i^\alpha$, $L(V_j^\alpha) = V_v^\beta$ such that $(v \in D_j) \wedge (V_v^\beta \in A_u^\beta)$, and
—$L(V_j^\alpha) \neq L(V_k^\alpha)$ for all $V_j^\alpha, V_k^\alpha$ in $A_i^\alpha$ such that $j \neq k$.

Here, *"L"* stands for *local*: the function $L$ involves an *allDifferent* constraint that is local in that it is restricted to $A_i^\alpha$. Indeed $L$ is the restriction of $I$ to $A_i^\alpha$. If no such function $L$ exists, then no function $I$ exists such that $I(V_i^\alpha) = V_u^\beta$, and in this case, $u$ can be removed from domain $D_i$. Solnon [2010] seeks a function $L$ by incremental application of the bipartite matching algorithm of Hopcroft and Karp [1973]. For each $(i, u)$, the worst-case complexity is $O(|A_i^\alpha| \times |A_u^\beta|)$.

Algorithms in Section 6.3 certainly ensure that all values in a solution are different without applying the local *allDifferent* constraint. For each $(i, u)$, the complexity of these bit-vector procedures is $O(|A_i^\alpha|)$ for

**for each** $j \in A_i^\alpha$ **do if** $D_j \cap M_j^i[u] = \emptyset$ **then** ...

[13]When used before focus search, BVCR preprocessing is implemented using linked-list instead of array representation of domains, because this is appreciably faster when there is no save/restore.

```
procedure prematches(in i, u: integer): boolean;
input:    i and u identify vertices in G^α and G^β respectively;
output:   the predicate prematches returns true if V_u^β could
          correspond to V_i^α in a subgraph isomorphism;
begin
    if degreeOf(V_i^α) > degreeOf(V_u^β) then return false end if;
    for k := 1 to degreeOf(V_i^α) do
      if degreeOf(V_{i_k}^α) > degreeOf(V_{u_k}^β) then return false end if;
    end for;
    return true
end prematches;
```

Fig. 8. Predicate *prematches* for undirected unlabeled graphs. This requires vertices in $A_i^\alpha$ and $A_u^\beta$ to be in sequence of decreasing degree.

but, without applying the local *allDifferent* constraint, we may remove fewer values from domains than does Solnon's process and, therefore, explore more combinations of values. This provides another example of a trade-off between doing more work after each elective instantiation, or instead doing less work but requiring more elective instantiations.

Instead of seeking a function $L$, Larrosa and Valiente [2002] apply a necessary but not sufficient condition for existence of a function $L$. The effect is to do less work than Solnon [2010] after each elective instantiation but remove fewer values from domains. Compared with our bit-vector procedures, Larrosa and Valiente may remove more values from domains but without the advantage of bit-parallel $D_j \cap M_j^i[u]$ in the innermost loop of the algorithm.

*6.4.2. Prematching.* Before preprocessing and search, when domains are such that

$$u \in D_i = (degreeOf(V_i^\alpha) \leq degreeOf(V_u^\beta))$$

a function $L$ can be sought by the very simple predicate procedure in Figure 8, which has time complexity $O(|A_i^\alpha|)$. This works correctly only if the vertices in

$$A_i^\alpha = \left\{ V_{i_1}^\alpha, \ldots, V_{i_k}^\alpha, \ldots, V_{i_{degreeOf(V_i^\alpha)}}^\alpha \right\}$$

have been sorted into sequence of decreasing degree and the vertices in

$$A_u^\beta = \left\{ V_{u_1}^\beta, \ldots, V_{u_k}^\beta, \ldots, V_{u_{degreeOf(V_u^\beta)}}^\beta \right\}$$

have also been sorted into this sequence. To see this, note that if $degreeOf(V_{i_1}^\alpha) > degreeOf(V_{u_1}^\beta)$, then no function $L$ exists because $V_{u_1}^\beta$ is the vertex in $A_u^\beta$ that has the largest degree. If $degreeOf(V_{i_1}^\alpha) \leq degreeOf(V_{u_1}^\beta)$, then *prematches* associates $V_{u_1}^\beta$ with $V_{i_1}^\alpha$ because there is no other member of $A_i^\alpha$ that has higher degree than $V_{i_1}^\alpha$ and should therefore be associated with $V_{u_1}^\beta$. If $degreeOf(V_{i_2}^\alpha) > degreeOf(V_{u_2}^\beta)$, then no function Ł exists because $V_{u_2}^\beta$ is the member of $\{V_{u_2}^\beta, \ldots, V_{u_{degreeOf(V_u^\beta)}}^\beta\}$ that has highest degree and $V_{u_1}^\beta$ is not available because it has already been associated with $V_{i_1}^\alpha$. Similar reasoning can be applied successively to the remaining members of $A_i^\alpha$.

The predicate *prematches* compares vertex invariants. For each vertex, the invariant is the degree of the vertex together with an ordered list of degrees of adjacent vertices. This is one of the first vertex invariants in a succession employed by Zampelli et al. [2010]. The next in this succession is the degree of the vertex together with, for each

```
procedure prematches(in i, u: integer): boolean;
input:   i and u identify vertices in G^α and G^β, respectively;
output:  the predicate prematches returns true if V_u^β could
           correspond to V_i^α in a subgraph isomorphism;
begin
    if (outDegreeOf(V_i^α) > outDegreeOf(V_u^β))) or
      (inDegreeOf(V_i^α) > inDegreeOf(V_u^β)) then  return false
    end if;
    for k := 1 to outDegreeOf(V_i^α) do
      if degreeOf(→V_{i_k}^α) > degreeOf(→V_{u_k}^β) then return false end if;
    end for;
    for k := 1 to inDegreeOf(V_i^α) do
      if degreeOf(←V_{i_k}^α) > degreeOf(←V_{u_k}^β) then return false end if;
    end for;
    return true
end prematches;
```

Fig. 9. Predicate *prematches* for directed unlabeled graphs. This requires that vertices adjacent to $V_i^\alpha$ and $V_u^\beta$ must be in sequence of decreasing degree.

adjacent vertex $V_a$, the degree of $V_a$ and an ordered list of degrees of vertices adjacent to $V_a$. Zampelli et al. continue this succession until it yields no further domain reduction.

In what follows, *prematching* means removing from each domain $D_i$ each value $u$ such that *prematches*$(i, u) =$ **false**. For initial domain reduction, before preprocessing and search, prematching usually turns out to be so cost-efficient that we will formulate versions of it for directed and for labeled subgraph isomorphism.

### 6.5. Directed Unlabeled Graphs

In a directed graph, an edge, which in this context is known as an *arc*, is an ordered pair of vertices; $(V_i^\alpha \rightarrow V_j^\alpha)$ denotes an arc from $V_i^\alpha$ to $V_j^\alpha$. When directed subgraph isomorphism is formulated as a constraint satisfaction problem, there is a binary constraint corresponding to every arc in $G^\alpha$. For an arc $(V_i^\alpha \rightarrow V_j^\alpha)$, the constraint predicate is $P_{i,j}(u, v) = (V_u^\beta \rightarrow V_v^\beta) \in E^\beta$ and the bit matrix $M_j^i$ is such that $M_j^i[u] = \{v|(V_u^\beta \rightarrow V_v^\beta) \in E^\beta\}$. For an arc $(V_i^\alpha \rightarrow V_j^\alpha)$, the constraint satisfaction algorithms in Section 3 require the asymmetric matrix $M_j^i$ and also its transpose $M_i^j$. This pair of matrices is the same for all $(i, j)$ such that $(V_i^\alpha \rightarrow V_j^\alpha) \in E^\alpha$. For an arc $(V_h^\alpha \leftarrow V_k^\alpha)$, the constraint satisfaction algorithms in Section 3 require the asymmetric matrix $M_k^h$ such that $M_k^h[u] = \{v|(V_u^\beta \leftarrow V_v^\beta) \in E^\beta\}$ and also its transpose $M_h^k$. Again, this pair of matrices is the same for all $(h, k)$ such that $(V_h^\alpha \leftarrow V_k^\alpha) \in E^\alpha$. Thus, for directed unlabeled graphs the overall total number of matrices required is four.

The *indegree* of a vertex is the number of arcs directed toward that vertex; the *outdegree* is the number of arcs directed away from that vertex. For directed subgraph isomorphism, we can apply unary constraints that allow $u \in D_i$ only if the indegree of $V_u^\beta$ is not less than the indegree of $V_i^\alpha$ and also the outdegree of $V_u^\beta$ is not less than the outdegree of $V_i^\alpha$. Figure 9 shows a version of the predicate *prematches* that enforces stronger unary constraints, which may eliminate more values from domains. For this, we define

$$\overrightarrow{A_i^\alpha} = \left\{V_j^\alpha | (V_i^\alpha \rightarrow V_j^\alpha) \in E^\alpha\right\}$$

Table I. Example of Indegrees and Outdegrees of Four Vertices Adjacent to $V_i^\alpha$ and $V_u^\beta$

| $\overrightarrow{A_i^\alpha}$ | | $\overrightarrow{A_u^\beta}$ | |
|---|---|---|---|
| indegree | outdegree | indegree | outdegree |
| 4 | 2 | 4 | 3 |
| 3 | 2 | 3 | 4 |
| 2 | 4 | 3 | 2 |
| 2 | 3 | 2 | 3 |

and

$$\overrightarrow{A_i^\alpha} = \left\{ \overrightarrow{V_{i_1}^\alpha}, \ldots, \overrightarrow{V_{i_k}^\alpha}, \ldots, \overrightarrow{V_{i_{outDegreeOf(V_i^\alpha)}}^\alpha} \right\}$$

in which the vertices have been sorted into sequence of decreasing degree, where $degree = indegree + outdegree$. We define $\overleftarrow{A_i^\alpha}$, $\overrightarrow{A_u^\beta}$ and $\overleftarrow{A_u^\beta}$ similarly.

An example in Table I illustrates what happens if we compare indegrees and outdegrees instead of simply comparing degrees in the last two loops in Figure 9. In this example, there are four vertices in $\overrightarrow{A_i^\alpha}$ and also in $\overrightarrow{A_u^\beta}$; Table I shows their indegrees and outdegrees. We seek a function $\vec{L} : \overrightarrow{A_i^\alpha} \rightarrow \overrightarrow{A_u^\beta}$ such that for all $k$ in $1, \ldots, 4$

—inDegreeOf($\overrightarrow{V_{i_k}^\alpha}$) $\leq$ inDegreeOf($\vec{L}(\overrightarrow{V_{i_k}^\alpha})$) *and*
—outDegreeOf($\overrightarrow{V_{i_k}^\alpha}$) $\leq$ outDegreeOf($\vec{L}(\overrightarrow{V_{i_k}^\alpha})$) *and*
—$\vec{L}$ satisfies the *allDifferent* constraint.

For this example, there is no lexicographic ordering on (indegree, outdegree) pairs in $\overrightarrow{A_i^\alpha}$ and in $\overrightarrow{A_u^\beta}$ such that a function $\vec{L}$ exists if and only if for all $k$ in $1, \ldots, 4$

$$\left(\text{inDegreeOf}(\overrightarrow{V_{i_k}^\alpha}) \leq \text{inDegreeOf}(\overrightarrow{V_{u_k}^\beta})\right) \textit{and} \left(\text{outDegreeOf}(\overrightarrow{V_{i_k}^\alpha}) \leq \text{outDegreeOf}(\overrightarrow{V_{u_k}^\beta})\right)$$

For the example in Table I, a function $\vec{L}$ does exist but finding it requires a process that has worst-case time complexity greater than $O(|\overrightarrow{A_i^\alpha}|)$.

### 6.6. Labeled Undirected Graphs

Vertices and edges may be labeled with information of any kind whatsoever. For example, labels may be numbers, or characters, or vectors, or sets. We now seek subgraph isomorphisms, $I$, such that

—attributeOf($I(V_i^\alpha)$) = attributeOf($V_i^\alpha$) **and**
—$(V_i^\alpha, V_j^\alpha) \in E_\alpha \Rightarrow (I(V_i^\alpha), I(V_j^\alpha)) \in E_\beta$ **and**
attributeOf($I(V_i^\alpha), I(V_j^\alpha)$) = attributeOf($V_i^\alpha, V_j^\alpha$) **and**
—$i \neq j \Rightarrow (I(V_i^\alpha) \neq I(V_j^\alpha))$

In molecule-matching applications [Willett 1999] attributes of vertices are letters that identify atoms (e.g., "C", "H", "O") and attributes of edges are bond-types, e.g., single, double, or aromatic. In the present section we insist, for simplicity, that attributes match exactly, although a more general requirement is that a predicate whose arguments may include attributes of $V_i^\alpha$ and $I(V_i^\alpha)$ returns **true** when there is a match within prescribed tolerances [Proschak et al. 2007].

When edges are not labeled, we have $M[u] = \{v | (u, v) \in E^\beta\}$, as in Section 6.1. When edges are labeled, more than one edge in $E^\alpha$ may have the same attribute. Let $\lambda_1, \ldots, \lambda_h, \ldots, \lambda_\eta$ be the set of distinct edge attributes that occur in $E^\alpha$. For an edge $(i, j)$ in $E^\alpha$ that has edge-attribute $\lambda_h$, and for the case where exact match is required,

the constraint predicate is

$$P_h(u, v) = ((u, v) \in E^\beta) \wedge \text{ attributeOf}(u, v) = \lambda_h),$$

and this is represented by a bit-matrix $M_h[u] = \{v | P_h(u, v)\}$. Thus, we require $\eta$ distinct bit-matrices, one for each distinct edge-attribute that occurs in $E^\alpha$. For each edge in $E^\alpha$, a domain reduction procedure such as BVCR now works with whichever bit-matrix has the same attribute as that edge. The binary constraint predicates are symmetric, so each is represented by a single bit-matrix, and the total number of such matrices is $\eta$. In molecule matching applications, $\eta$ is usually very much less than the number of edges in $E^\alpha$, indeed often less than eight.

We take the liberty of saying that vertex $V_j$, adjacent to vertex $V_i$, has edge-attribute $\lambda_h$, meaning that the edge $(i, j)$ has edge-attribute $\lambda_h$. Let $\nu_1, \ldots, \nu_k, \ldots, \nu_\zeta$ be the set of different vertex attributes that occur in $V^\alpha$. We define the *hk*-attribute-degree of vertex $V_i$ to be the number of vertices $V_j$ adjacent to $V_i$ such that $V_j$ has edge-attribute $\lambda_h$ and vertex-attribute $\nu_k$. It is reasonable to include $u \in D_i$ only if for all $h \in [1, \ldots, \eta]$ and for all $k \in [1, \ldots, \zeta]$ the *hk*-attribute-degree of vertex $V_i^\alpha$ is not greater than the *hk*-attribute-degree of a vertex $V_u^\beta$.

Going further, the version of predicate *prematches* in Figure 11 applies the local *allDifferent* constraint. For each *hk* pair, this version of *prematches* seeks correspondence between degrees of individual adjacent variables. Before the first call of *prematches*, we construct a separate triple list structure for each vertex. This vertex invariant structure is of the same type for every vertex in $V^\alpha$ and in $V^\beta$, and remains unchanged during all invocations of *prematches*. This structure is now described for a vertex $V_i$.

For $V_i$, there is an outer list that has one member for each different edge attribute of any vertex adjacent to $V_i$. The member of this list for edge attribute $\lambda_h$ points to a further list that has one member for each different vertex attribute of any vertex adjacent to $V_i$ that has edge attribute $\lambda_h$. The member of this further list that corresponds to edge attribute $\lambda_h$ and vertex attribute $\nu_k$ points to a final list that has one member for each vertex (adjacent to $V_i$) that has edge attribute $\lambda_h$ and vertex attribute $\nu_k$. In this final list, the member for each vertex $V_j$ includes the degree of $V_j$. Every final list must be in sorted order of decreasing degree; more than one vertex in a final list may have the same degree. There are no duplicates in the outermost list and in the middle lists, which must be in a sorted order that is the same for all vertices. These lists are here assumed to be in decreasing sequence of attribute value.[14] Figure 10 shows the list structure for an example in which the (edge-attribute, vertex-attribute) pairs for the ten vertices adjacent to $V_i$ are (4, 3), (4, 1), (3, 6), (1, 5), (1,3), (1, 1). In practice, many final lists have only one member.

In Figure 11 the loop at Lines 24 through 30 simply compares degrees. To compare *hk*-attribute-degrees instead, we would require an algorithm that has non-linear time complexity, for the reason that was illustrated by the example in Table I. However, there is no problem when the loop at Lines 23 through 29 is amended to compare distance-2-degrees instead of distance-1-degrees.

When a single graph $G^\alpha$ is compared with a single graph $G^\beta$, the memory occupied by the lists can be released after the initial membership of domains has been determined. In systems that have dynamic memory allocation, this area of memory can be reused for bit-matrices, which can be constructed after all unary constraints have been applied.

[14]When these attributes are letters such as "C," "H," "O," a list is sorted in decreasing sequence of ordinals uniquely associated with letters. This association must be the same for all vertices.

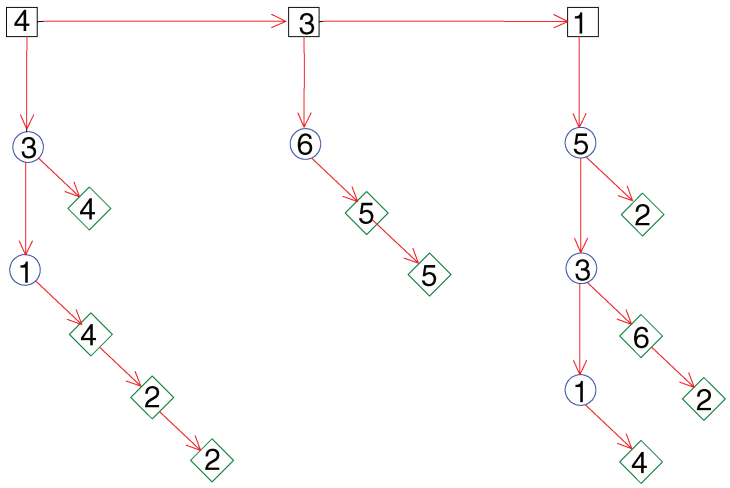



Fig. 10. Triple list structure. Numbers in the horizonal list are edge attribute values. Numbers in vertical lists are vertex attribute values. Numbers in diagonal lists are degrees of individual vertices.

### 6.7. Graph Retrieval

Most practical applications of subgraph isomorphism involve comparison of many pairs of graphs. In image-matching applications, many small graphs are compared with a single bigger graph [Conte et al. 2004]. Contrariwise, in chemical applications [Brown 2009; Willett 1999], a single molecular substructure is compared with many bigger molecules. More generally, graph retrieval is concerned with a large collection of graphs, which are known in this context as *targets*. Given a smaller graph, here known as a *query*, a common practical requirement is to identify all targets to which the query is subgraph isomorphic [Cheng et al. 2009; Zou et al. 2008]. A more general requirement, which is not addressed in this article, is to find all targets to which the query is approximately subgraph isomorphic [Yan et al. 2006].

The simple routine

**for** each target **do** seek subgraph isomorphism between query and target

would usually be intolerably slow. Instead, normal practice is to employ a set, sometimes known as an *alphabet*, of small subgraphs, known as *fragments*. We identify all fragments that are in the query and also in the alphabet, and we do the same for every target. For the set of targets, this information can be reused for any number of queries. If the set of fragments in a given target does not include the set of fragments in the query, then the query cannot possibly be subgraph isomorphic to this target, and a search for isomorphism should, therefore, be omitted. The alphabet of fragments is chosen with the aim of maximizing avoidance of fruitless searches.

For each fragment in the alphabet, Yan et al. [2005] compile an index list of (identifiers of) all target graphs that include this fragment. Yan et al. seek detailed subgraph isomorphism between the query and each of the target graphs within the intersection of the index lists for those fragments that are included in the query. If the indexed fragments are small, then we may need many of them, each associated with a list of many thousands of target identifiers. Intersecting many long lists takes considerable time. Having larger fragments in the alphabet can reduce the length of these lists, but the number of possible fragments increases exponentially with their size [Jiang et al. 2007].

```
procedure prematches(in i, u : integer): boolean;
input:   i and u identify vertices in G^α and G^β, respectively;
output:  the predicate prematches returns true if V_u^β could
           correspond to V_i^α in a subgraph isomorphism;
begin
1   if vertexAttributeOf(V_i^α) ≠ vertexAttributeOf(V_u^β) then return false end if
2   alphaEdgePtr:= pointerToFirstRecordInListOfEdgeAttributesOf V_i^α;
3   betaEdgePtr:= pointerToFirstRecordInListOfEdgeAttributesOf V_u^β;
4   while alphaEdgePtr ≠ nil do (* iterate over edge attributes *)
5     loop (* to find identical edge attributes *)
6       if (betaEdgePtr = nil) or
7         betaEdgePtr↑.attribute < alphaEdgePtr↑.attribute) then return false
8       elsif betaEdgePtr↑.attribute = alphaEdgePtr↑.attribute then exit
9       else betaEdgePtr:= betaEdgePtr↑.next
10      end if
11    end loop;
12    alphaVertexPtr:= alphaEdgePtr↑.pointerToFirstRecordInListOfVertexAttributes;
13    betaVertexPtr:= betaEdgePtr↑.pointerToFirstRecordInListOfVertexAttributes;
14    repeat (* iterate over vertex attributes *)
15      loop (* to find identical vertex attributes *)
16        if (betaVertexPtr = nil) or
17          (betaVertexPtr↑.attribute < alphaVertexPtr↑.attribute) then return false
18        elsif betaVertexPtr↑.attribute = alphaVertexPtr↑.attribute then exit
19        else betaVertexPtr:= betaVertexPtr↑.next
20        end if
21      end loop;
22      alphaDegreePtr:= alphaVertexPtr↑.pointerToFirstRecordInListOfVertices;
23      betaDegreePtr:= betaVertexPtr↑.pointerToFirstRecordInListOfVertices;
24      loop (* comparing degrees of individual adjacent vertices *)
25        if alphaDegreePtr↑.degree > betaDegreePtr↑.degree then return false end if;
26        alphaDegreePtr:= alphaDegreePtr↑.next;
27        if alphaDegreePtr = nil then exit end if
28        betaDegreePtr:= betaDegreePtr↑.next;
29        if betaDegreePtr = nil then return false end if
30      end loop; (* over individual vertices *)
31      alphaVertexPtr:= alphaVertexPtr↑.next;
32    until alphaVertexPtr = nil;
33    alphaEdgePtr:= alphaEdgePtr↑.next;
34  end while;
35  return true
end prematches
```

Fig. 11. Predicate *prematches* for labeled undirected graphs.

The use of signatures is a well-established alternative to the use of indexes. The simplest *bit-string* method associates with each target, and also with a query, a bit-vector in which there is one bit corresponding to each fragment in the alphabet [Willett 2005]. These bit-vectors typically comprise 1,000 bits. In a target's bit-vector, a bit is "1" if and only if the corresponding fragment is in the target. Similarly, in a query bit-vector a bit is "1" if and only if the corresponding fragment is in the query. If bit-parallel operations reveal that any "1" in the query bit-vector corresponds to a "0" in a target bit-vector, then isomorphism between the query and this target should not be

```
for each target do
  for each trilabel in the query do
    if the number of occurrences in the query does not exceed the
      number of occurrences of this trilabel in the target then
      if prematching does not empty any domain then
        if preprocessing does not empty any domain then
          seek subgraph isomorphism between query and target
```

Fig. 12. Brief outline of graph retrieval procedure.

sought. In this context, a bit-vector is an example of a *signature*, that is, a collection of information that characterizes a target.

For textual information retrieval, Zobel et al. [1998] found that index-based methods substantially outperformed signature methods. However, the number of fragments involved in a conjunctive graph retrieval query is usually not so small. This is one reason why, for graph retrieval, bit-vector methods are well established in practice [Daylight Chemical Information Systems, Inc. 2007], whereas index-based methods are still subject to research investigation [Zhang et al. 2009; Zhao et al. 2007; Cheng et al. 2009].

Fragment-based methods require judicious selection of the alphabet. Selection requires substantial effort, which may need to be repeated for each different collection of targets. Moreover, detection of selected fragments within a query may take appreciable time. These disadvantages can be avoided by using a signature method with very simple fragments, and counting their occurrences instead of merely detecting their presence or absence. More specifically, following Chang and Lee [1991], our experiments work with trilabels.

A *trilabel* is a triple comprising the label of a vertex, the label of an adjacent vertex, and the label of the edge between these two vertices. A trilabel, which is the same thing as a *2-graph* [Chou and Shapiro 1998] and a *distinct edge* [Cheng et al. 2009] is analogous to a textual trigram. Prior to retrieval, we store, for each target graph, a signature which consists of the number of occurrences of each and every trilabel in that target. Signatures can subsequently be used in answering any number of queries. At query time, we count the number of occurrences of each and every trilabel in the query and then proceed as in Figure 12. For each trilabel in the query signature, this routine requires a search for the same trilabel in the target signature. Appendix Section D describes a fast trilabel matching procedure.

As in Graph Grep [Giugno and Shasha 2002; Shasha et al. 2002], paths of length greater than one could be used instead of trilabels, but of course the number of paths increases rapidly with their length. Instead of using longer paths, we rely on prematching and preprocessing to reduce the number of searches for subgraph isomorphism. Prematching and preprocessing achieve domain reduction that facilitates search, whereas trilabel matching does not. The trilabel test simply prevents further work on comparisons that can certainly not yield any isomorphism. Another comment is that neither prematching nor preprocessing has worst-case exponential time complexity.

## 7. EXPERIMENTS

### 7.1. Experiments with Randomly Generated Constraint Satisfaction Problems

*7.1.1. Experimental Framework.* Section 7.1 reports experiments with randomly generated instances of the general binary constraint satisfaction problem, not with isomorphism. Parameters that characterize an instance are

$n$, the number of variables.

$e$, the number of scopes. A *scope* is a set of variables that are all subject to the same constraint.
$\rho$, the average degree of the variables: $\rho = 2e/n$. The degree of a variable $V_i$ is the number of variables to which $V_i$ is adjacent.
$\delta$, the domain cardinality. Every domain has the same cardinality $\delta$.
$J$, the number of $(u, v)$ pairs such that $P_{ij}(u, v) =$ **true**. $J$ is the same for each pair $(i, j)$ of variables that are subject to a constraint. In other words, every scope has the same $J$.

Exponential time complexity implies that there is a region, within the space defined by these parameters, where algorithms are too slow to be serviceable. A central purpose of our experiments is to explore the extent of this region on a larger scale than has been reported previously. A further purpose is to compare performance of algorithms. With randomly generated instances, we can observe and compare algorithm performance when parameters $n$, $\rho$, $\delta$ and $J$ are varied systematically, but we cannot explore the whole of this four-dimensional space. Instead, we have chosen combinations of parameter values to illustrate their effect on the relative speed of algorithms.

We generate random instances by first choosing $e = n\rho/2$ scopes randomly, except we make the degree of every variable be at least two, to prevent a short cut that saves time by processing acyclic subgraphs after cyclic parts of the constraint network have been satisfied [Sabin and Freuder 1997]. Moreover, we do not use any randomly chosen set of scopes that does not have a connected constraint graph. This prevents replacement of the constraint satisfaction by a collection of separate smaller problems.

After choosing scopes, our generator randomly chooses $J$ pairs of values on each scope. No two pairs of values on the same scope are the same: Duplicates are precluded. If $R_{ij}$ is the set of randomly chosen tuples (i.e., pairs of values) on the scope $(i, j)$, then $P_{ij}(u, v) \equiv (u, v) \in R_{ij}$ and $J = |R_{ij}|$. Except for making the degree of every variable be at least two, our generator is the same as the Model B generator [Gent et al. 2001]. Constraints generated in this way are asymmetric: $P_{i,j}(u, v) \not\equiv P_{i,j}(v, u)$.

For each of the randomly chosen scopes, the set of randomly chosen pairs of values on that scope is put directly into fast main memory (not disk) by the random generator. Timings reported in the following are initialized when this has been done. These timings, using a 3.2GHz Pentium 4 with 2GB of RAM, include time for initialization of the bit matrices. In Sections 7.1.2 and 7.2, the search stops as soon as a solution is found. Constraints are randomly generated completely afresh for each trial. Many trials are required when variance of time taken is high.

In Section 7.1, algorithms are identified as follows, always without preprocessing, always with pop-stack restoration and always with duplicate representation of domains except in Tables II and III

*BVDR:* Bit-vector direct reduction, as in Sections 3.2 and B.2.
*BVCR:* Bit-vector cumulative reduction, as in Sections 3.3 and B.2.
*BVFC:* Bit-vector forward checking, as in Sections 3.4 and B.2.
*Focus:* Focus search, as in Section 4.
*AC2001:* As in Bessière et al. [2005].

Tables II and III show that in some cases duplicate (i.e., bit-vector and array) representation[15] makes the search somewhat slower. In Section 7.1.2, we have only used

[15]Duplicate representation is intended to save time by avoiding visiting 0's in bit-vectors. In Table II, duplicate representation is slowest when the average number of 0's in bit-vectors is highest, which is the opposite of what we expected.

Table II. The *ratio* column shows the time taken using duplicate representation of domains divided by the time taken using only bit-vector representation.

| | | | BVCR | | | BVDR | BVFC |
|---|---|---|---|---|---|---|---|
| $\rho$ | $n$ | $\delta$ | ratio | nb0s | depth | ratio | ratio |
| 3.5 | 100 | 300 | 1.294 | 104.71 | 2.02 | 1.373 | - |
| 7.0 | 100 | 100 | 0.713 | 34.58 | 2.36 | 0.836 | 0.915 |
| 7.0 | 100 | 300 | 1.336 | 92.74 | 1.68 | 1.431 | 1.125 |
| 7.0 | 300 | 100 | 0.978 | 22.71 | 2.38 | 1.059 | 1.096 |
| 7.0 | 300 | 300 | 1.380 | 65.52 | 1.77 | 1.549 | 0.986 |
| 14.0 | 300 | 100 | 1.003 | 21.47 | 2.05 | 1.088 | 1.011 |

With duplicate representation, the time is the average over all the trials in Figures 13, 14, 15 and 16. With only bit-vector representation, the time is the average over the same number of trials with the same parameters. The column headed *nb0s* shows the average number of 0's in bit-vectors immediately before invocation of the domain reduction procedure. The *depth* is the average number of electively instantiated variables at this time.

Table III. Cumulative Reduction with Higher $J$ than in Table II

| | | | | BVCR + Duplicate | | | | BVO | |
|---|---|---|---|---|---|---|---|---|---|
| $\rho$ | $n$ | $\delta$ | J | av | sd | nb0s | depth | av | sd |
| 3.5 | 100 | 300 | 4,600 | 4.60 | 1.91 | 224.5 | 13.4 | 6.65 | 0.75 |
| 7.0 | 100 | 100 | 3,225 | 1.32 | 0.21 | 87.6 | 27.6 | 3.25 | 0.56 |
| 7.0 | 100 | 300 | 22,900 | 2.12 | 0.41 | 280.5 | 35.9 | 3.19 | 0.73 |
| 7.0 | 300 | 100 | 3,380 | 2.22 | 0.74 | 89.4 | 92.7 | 1.44 | 0.20 |
| 7.0 | 300 | 300 | 23,600 | 4.99 | 1.65 | 275.4 | 108.2 | 4.01 | 1.10 |
| 14.0 | 300 | 100 | 6,024 | 2.53 | 0.25 | 95.7 | 130.3 | 5.35 | 0.97 |

Average times for 1,000 trials with duplicate representation of domains and also with only bit-vector representation (BVO). *sd* is the standard deviation of the average, not of the variate. Meanings of *nb0s* and *depth* are the same as in Table II.

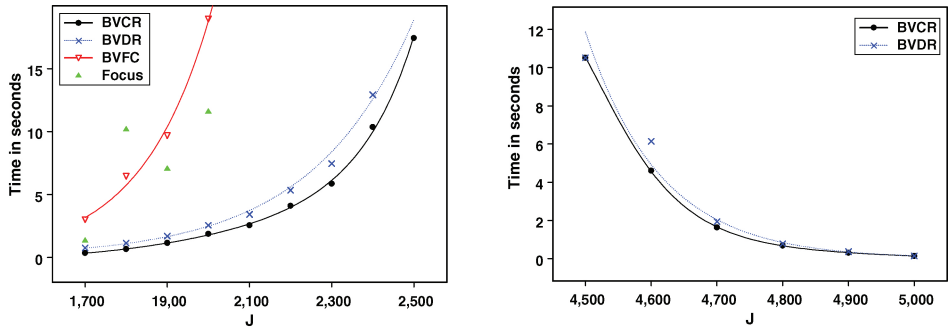
duplicate representation because switching between duplicate and bit-vector-only representation would obscure intercomparison of results.

*7.1.2. Examples of Time-Growth Curves.* As before, $J$ is the number of $(u, v)$ pairs such that $P_{ij}(u, v) = \mathbf{true}$; $\delta$ is the domain cardinality. When $J$ is small, the constraints are said to be *tight*. When $J$ is large in comparison with its maximum value, $\delta^2$, the constraints are said to be *loose*. A problem that has very tight constraints is unlikely to have any solution, whereas a problem with very loose constraints is unlikely not to have any solution. Between these extremes there is a well-known *crossover point* where the probability of existence of a solution is 0.5 and random problems require the largest search [Prosser 1996; Smith and Dyer 1996].

When $J$ increases in (a) in Figures 13, 14, 15, and 16, there is exponential growth of time on the tight side of crossover, where there is no solution. When $J$ increases above crossover, the number of solutions increases, so the time to find one decreases in (b) in these figures. Between (a) and (b) there is a gap, within the range of $J$, wherein exponential time complexity makes these algorithms impractical. In Table IV, this gap increases with the average degree $\rho$, because when there are more constraints, it is more difficult to find a solution on the loose side of crossover. The gap increases when *looseEnd* decreases.

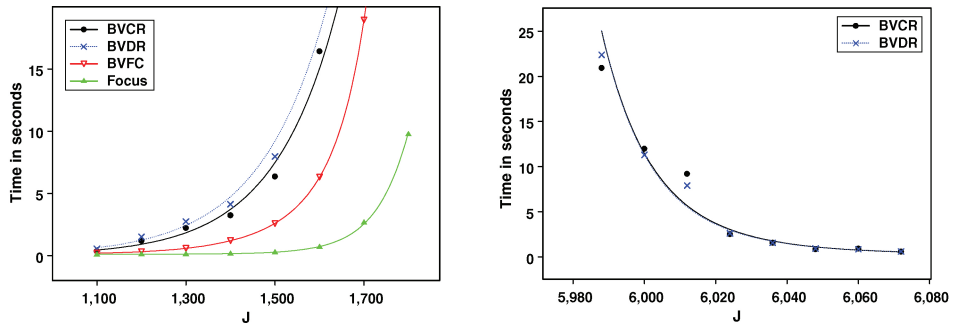
Comparing Figure 13(a) with Figure 15(c), also Figure 14(a) with Figure 16(a), we see that, on the tight side of crossover, search becomes much faster when $\rho$ is doubled and other parameters are unchanged. Search is faster because it is more constrained.[16]

[16]When constraints are not binary, search is faster the greater the number of variables within each constraint [Ullmann 2007, Table 9].




(a) (b)

Fig. 13. Average times versus $J$ in 1,000 trials with average degree $\rho = 3.5$, number of variables $n = 100$, and domain cardinality $\delta = 300$. (a) Tight side of crossover. (b) Loose side of crossover.




(a) (b)

Fig. 14. Average times versus $J$ with average degree $\rho = 14$, number of variables $n = 300$ and domain cardinality $\delta = 100$. (a) 500 trials on the tight side of crossover. (b) 1,000 trials on the loose side of crossover, where variance of average time is greater.

Table IV.

| Figure | $\rho$ | n | $\delta$ | gap | looseEnd |
|---|---|---|---|---|---|
| 13(a)(b) | 3.5 | 100 | 300 | 0.023 | 0.950 |
| 15(a)(b) | 7.0 | 100 | 100 | 0.162 | 0.682 |
| 15(c)(d) | 7.0 | 100 | 300 | 0.187 | 0.750 |
| 16(a)(b) | 7.0 | 300 | 100 | 0.230 | 0.666 |
| 16(c)(d) | 7.0 | 300 | 300 | 0.223 | 0.739 |
| 14(a)(b) | 14.0 | 300 | 100 | 0.446 | 0.400 |

$J_T = J$ such that the average BVCR search time on the tight side of crossover is 10 seconds. $J_L = J$ such that the average BVCR search time on the loose side of crossover is 10 seconds. $\delta$ is the maximum cardinality of domains; $\delta^2$ is the greatest possible value of $J$. Gap $= (J_L - J_T)/\delta^2$. LooseEnd $= (\delta^2 - J_L)/\delta^2$. Again, $\rho$ is the average degree; $n$ is the number of variables.

We also see that cumulative reduction is appreciably faster than direct reduction on the tight side, but there is no significant difference on the loose side of crossover. On the loose side, forward checking, focus search and AC2001 are always very much slower than cumulative reduction: Table V gives examples. On the tight side, AC2001 is always very much slower than direct reduction (BVDR), as would be expected from the wide-ranging large-scale experimental results of Lecoutre and Vion [2008]. Our subsequent experiments exclude AC2001 because there is no reason to expect it to be competitive with BVCR.

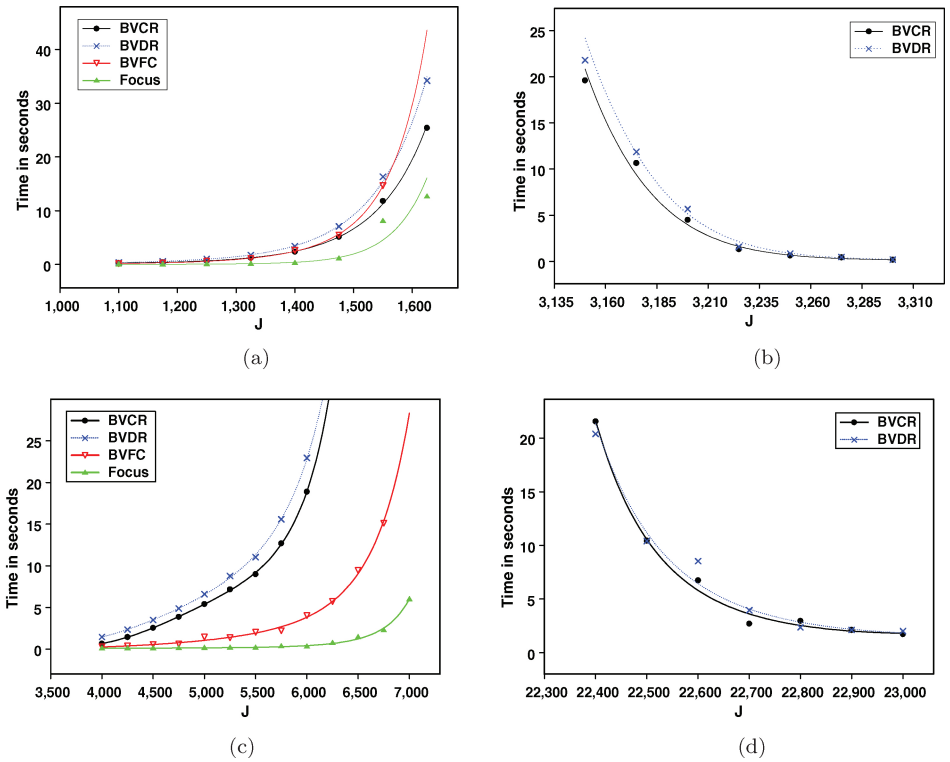



Fig. 15. Average times versus $J$ with average degree $\rho = 7$ and number of variables $n = 100$; (a) $\delta = 100$; 500 trials on the tight side of crossover. (b) $\delta = 100$; 1,000 trials on the loose side of crossover. (c) $\delta = 300$; 500 trials on the tight side of crossover. (d) $\delta = 300$; 1,000 trials on the loose side of crossover.

Table V. Average Time in Seconds, and Standard Deviation of Average Time, on the Loose Side of Crossover, with $\rho = 7$

| $n$ | $\delta$ | $J$ | Algorithm | Time Av | Time Sd | NbOfTrials |
|---|---|---|---|---|---|---|
| 100 | 100 | 3,300 | BVCR | 0.17 | 0.02 | 1,000 |
| 100 | 100 | 3,300 | BVFC | 4.15 | 0.94 | 100 |
| 100 | 100 | 3,300 | Focus | 101.96 | 32.98 | 100 |
| 100 | 100 | 3,300 | AC2001 | 12.42 | 0.52 | 100 |
| 100 | 300 | 23,000 | BVCR | 1.72 | 0.41 | 1000 |
| 100 | 300 | 23,000 | BVFC | 8.72 | 2.19 | 500 |
| 100 | 300 | 23,000 | Focus | 71.61 | 31.76 | 100 |
| 100 | 300 | 23,000 | AC2001 | 343.10 | 66.61 | 100 |
| 300 | 100 | 3,430 | BVCR | 0.20 | 0.01 | 1000 |
| 300 | 100 | 3,430 | BVFC | - | - | - |
| 300 | 100 | 3,430 | Focus | - | - | - |
| 300 | 100 | 3,430 | AC2001 | 188.96 | 71.13 | 50 |
| 300 | 300 | 23,700 | BVCR | 5.01 | 2.05 | 1000 |
| 300 | 300 | 23,700 | BVFC | 767.79 | 268.51 | 10 |
| 300 | 300 | 23,700 | Focus | - | - | - |
| 300 | 300 | 23,700 | AC2001 | 135.20 | 7.74 | 50 |

Here "-" signifies that the algorithm was too slow to permit sufficient trials. *NbOfTrials* is the number of trials.

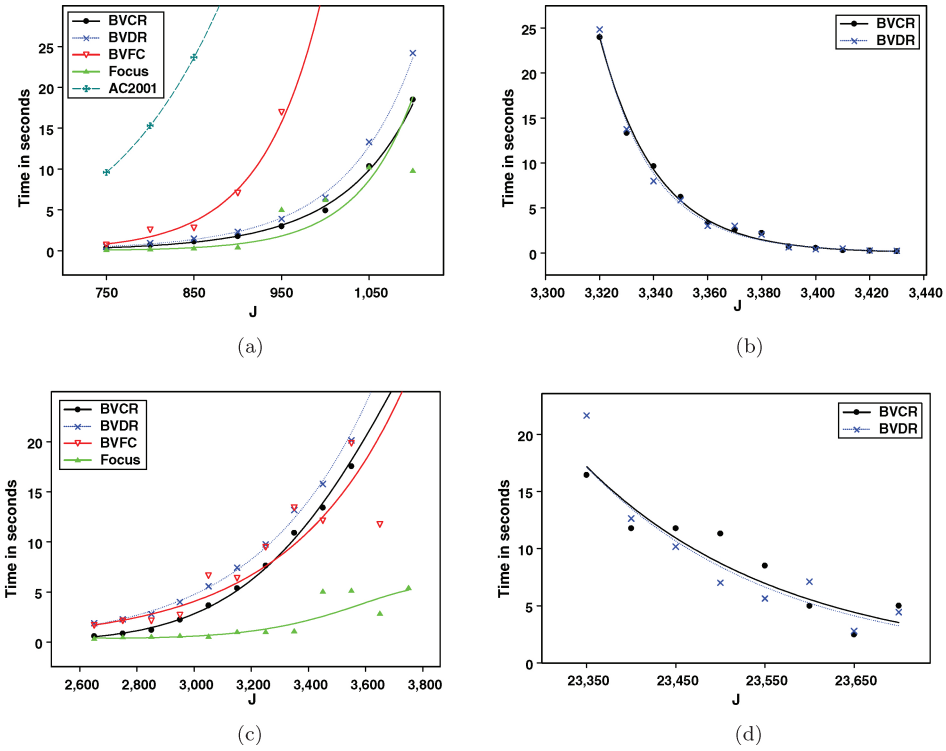



Fig. 16. Average times versus $J$ with average degree $\rho = 7$ and number of variables $n = 300$. (a) Domain cardinality $\delta = 100$; 500 trials on the tight side of crossover. (b) $\delta = 100$; 1,000 trials on the loose side of crossover. (c) $\delta = 300$; 500 trials on the tight side of crossover. (d) $\delta = 300$; 1,000 trials on the loose side of crossover.

Focus search time depends on the number values to which a variable will be instantiated. This is the number of 1's in the result of bit-vector intersection at Line 6 in Figure 6. Focus search becomes more competitive when this number is reduced:

*By increasing the average degree of variables.* This increases the number of bit-vectors that are intersected. Focus search is faster in Figure 15(c), where average degree $\rho = 7$, than in Figure 13(a), where $\rho = 3.5$. Again, focus search is faster in Figure 14, where $\rho = 14$, than in Figure 16(a), where $\rho = 7.0$, other parameters being the same.

*By increasing $\delta$ whilst $J$ remains unchanged.* This reduces the density of 1's in bit-matrix rows. Focus search is faster in Figure 15(c), where $\delta = 300$, than in Figure 15(a), where $\delta = 100$. Again, focus search is faster in Figure 16(c), where $\delta = 300$, than in Figure 16(a), where $\delta = 100$, other parameters being the same.

*By decreasing the average cardinality of domains.* Sections 7.6.4 and 7.7 provide examples.
It is not so easy to explain why focus search is less competitive in Figure 16(a), where $n = 300$, than in Figure 15(a), where $n = 100$.

### 7.2. Experiments with Frequency Assignment Problems

Binary constraint satisfaction problems arise in the assignment of frequency and polarization to radio links so as to satisfy constraints such as minimization of

interference [Aardal et al. 2007]. A collection of *fapp* (i.e., frequency assignment problem with polarization) problem instances are available at http://www.cril.univ-artois.fr/~lecoutre/research/benchmarks/benchmarks.html for use as benchmarks in the experimental evaluation of constraint satisfaction algorithms; physical requirements have been translated into clear ready-made constraint satisfaction problem formulations. An XML file includes, for each instance, a specification of the domains of variables, a specification of constraint scopes, and a specification of one or more numeric predicates that must be satisfied on each scope. An example of a numeric predicate is

$$P_{ij}(u, v) = (u \times v < a) \vee (|u - v| \geq b),$$

where $a$ and $b$ are prescribed constants.

These *fapp* benchmarks consist of forty sets, *fapp*01, *fapp*02..., *fapp*40, each containing eleven instances. Within each set, the eleven instances all have the same number, $n$, of variables, the same number, $e$, of scopes, and, for each domain, the same $upperBound - lowerBound$. In fact $upperBound - lowerBound$ is so big that bit-vector algorithms are practical only with surrogate values, as in Section 5. For example, for *fapp*01, the greatest range of values in any domain is 5,312, whereas $\delta = 190$. Another example is that for *fapp*20, the greatest range of values in any domain is 5,640, whereas $\delta = 302$. Within each set, all of the eleven instances have the same value of $\delta$.

In these *fapp* benchmarks, there are many cases where, for a given scope, two specified predicates must both be satisfied. If these two predicates for the scope $(i, j)$ are $P_{ij}^1$ and $P_{ij}^2$ then bit-matrices $M_j^i$ and $M_i^j$, initially empty, can be constructed by the routine

```
for each surrogate value u of V_i do
    for each surrogate value v of V_j do
        if P_ij^1(S_i(u), S_j(v)) ∧ P_ij^2(S_i(u), S_j(v)) then
            include v in M_j^i[u]; include u in M_i^j[v];
        end if
    end for
end for
```

In Table VI, differences in average timings for BVDR, BVCR, and IRCR may not be significant since there are only 11 instances in each of the 40 sets, so we have small-sample statistics. Because incremental restoration requires less memory, IRCR processes 55 more *fapp* instances than BVCR and BVDR. Another comment is that *Set-up time* is almost entirely the average time to construct bit-matrices. Although in most cases the set-up time very greatly exceeds the search time, the use of bit-matrices may nevertheless be sensible because set-up time is $O(e\delta^2)$ whereas a search algorithm has worst-case exponential time complexity. For the *fapp* benchmarks, timings obtained by other workers can be seen at http://www.cril.univ-artois.fr/CPAI06/round2/results/globalbybench.php?idev=6&idcat=38&idSubCat=56.

Table VII shows average search time and numbers of timeouts for forward checking (without preprocessing) on *fapp*01-10. Here, forward checking is certainly very much slower than BVCR. With focus search (without preprocessing), there is timeout on all of these 110 instances, so focus search is certainly very much slower than forward checking. Very poor timings for focus search and forward checking can probably be attributed to the looseness of the constraints, which was unhelpful to these procedures on the loose side of crossover in Section 7.1.

### 7.3. Graph Versions of Algorithms

The remainder of Section 7 deals with isomorphism, for which search is always preceded by preprocessing. Algorithms are henceforward identified as follows.

Table VI. Parameters and Timings on $40 \times 11$ *fapp* Instances, Using Duplicate Representation of Domains, Not Using Preprocessing, and Stopping When One Solution Is Found

| | | | | Set-up | BVDR | | BVCR | | IRCR | |
|---|---|---|---|---|---|---|---|---|---|---|
| fapp | $n$ | $e$ | $\delta$ | time | time | to | time | to | time | to |
| 01 | 200 | 1,108 | 190 | 8.71 | 0.283 | 0 | 0.225 | 0 | 0.222 | 0 |
| 02 | 250 | 1,636 | 210 | 16.02 | 0.345 | 0 | 0.277 | 0 | 0.283 | 0 |
| 03 | 300 | 2,327 | 250 | 35.35 | 0.244 | 0 | 0.254 | 0 | 0.254 | 0 |
| 04 | 300 | 1,799 | 270 | 35.49 | 4.045 | 0 | 4.911 | 0 | 4.961 | 0 |
| 05 | 350 | 2,488 | 270 | 59.46 | 0.792 | 0 | 0.772 | 0 | 0.774 | 0 |
| 06 | 500 | 3,478 | 290 | 78.93 | 7.142 | 0 | 7.618 | 0 | 7.618 | 0 |
| 07 | 600 | 4,777 | 302 | 79.49 | 0.410 | 0 | 0.346 | 0 | 0.348 | 0 |
| 08 | 700 | 3,834 | 282 | 71.38 | 1.264 | 0 | 1.535 | 0 | 1.371 | 0 |
| 09 | 800 | 4,800 | 350 | 61.08 | 0.634 | 0 | 1.097 | 0 | 1.078 | 0 |
| 10 | 900 | 6,071 | 362 | 164.21 | 2.541 | 0 | 1.944 | 0 | 1.940 | 0 |
| 11 | 1,000 | 8,005 | 362 | 319.38 | 2.335 | 0 | 42.780 | 0 | 42.700 | 0 |
| 12 | 1,500 | 13,439 | 310 | 506.64 | 19.845 | 6 | 59.992 | 5 | 59.527 | 5 |
| 13 | 2,000 | 13,699 | 190 | 156.47 | 4.507 | 4 | 4.476 | 4 | 4.538 | 4 |
| 14 | 2,500 | 21,610 | 362 | 942.23 | - | - | - | - | 143.328 | 6 |
| 15 | 3,000 | 17,754 | 182 | 218.08 | 13.309 | 1 | 1.603 | 2 | 1.595 | 2 |
| 16 | 260 | 2,088 | 302 | 29.96 | 0.007 | 0 | 0.003 | 0 | 0.012 | 0 |
| 17 | 300 | 2,056 | 302 | 40.24 | 0.014 | 0 | 0.010 | 0 | 0.017 | 0 |
| 18 | 350 | 2,387 | 302 | 34.93 | 0.012 | 0 | 0.011 | 0 | 0.021 | 0 |
| 19 | 350 | 3,114 | 802 | 515.94 | 0.149 | 0 | 0.127 | 0 | 0.114 | 0 |
| 20 | 420 | 2,487 | 302 | 51.03 | 0.009 | 0 | 0.009 | 0 | 0.011 | 0 |
| 21 | 500 | 1,589 | 242 | 30.31 | 0.056 | 0 | 0.046 | 0 | 0.108 | 0 |
| 22 | 1,750 | 16,924 | 802 | - | - | - | - | - | - | - |
| 23 | 1,800 | 33,337 | 302 | 859.99 | 0.048 | 0 | 0.059 | 0 | 0.049 | 0 |
| 24 | 2,000 | 14,301 | 302 | 453.17 | 0.219 | 0 | 0.189 | 0 | 0.184 | 0 |
| 25 | 2,230 | 11,974 | 302 | 266.76 | 0.193 | 0 | 0.154 | 0 | 0.155 | 0 |
| 26 | 2,300 | 12,761 | 302 | 386.77 | 0.335 | 0 | 0.334 | 0 | 0.255 | 0 |
| 27 | 2,550 | 6,231 | 242 | 117.77 | 0.753 | 0 | 0.636 | 0 | 0.632 | 0 |
| 28 | 2,800 | 12,046 | 998 | - | - | - | - | - | - | - |
| 29 | 2,900 | 41,781 | 998 | - | - | - | - | - | - | - |
| 30 | 3,000 | 33,301 | 778 | - | - | - | - | - | - | - |
| 31 | 400 | 1,644 | 700 | 280.97 | - | - | - | - | 1.060 | 0 |
| 32 | 550 | 5,017 | 998 | - | - | - | - | - | - | - |
| 33 | 650 | 4,631 | 498 | 288.29 | - | - | - | | 0.142 | 0 |
| 34 | 750 | 4,623 | 998 | - | - | - | - | - | - | - |
| 35 | 1,500 | 11,723 | 698 | - | - | - | - | - | - | - |
| 36 | 2,000 | 10,067 | 454 | 517.94 | - | - | - | - | 0.445 | 0 |
| 37 | 2,250 | 22,553 | 998 | - | - | - | - | - | - | - |
| 38 | 2,500 | 32,622 | 698 | - | - | - | - | - | - | - |
| 39 | 2,750 | 12,605 | 502 | 1,115.05 | - | - | - | - | 2.829 | 0 |
| 40 | 3,000 | 28,313 | 698 | - | - | - | - | - | - | - |

BVDR and BVCR use pop-stack domain restoration; IRCR differs from BVCR only in that it uses incremental restoration. If the search takes more than 1,000 seconds it is stopped and this situation is a *timeout*; *"to"* denotes the number of timeouts; *time* is the average search time. This is the average over only those instances for which there is no timeout. "-" signifies insufficient memory.

*BVCR:* Bit-vector cumulative reduction, as in Section 6.3.1,
*BVFC:* Bit-vector forward checking, as in Section 6.3.2,
*Focus:* Focus search, as in Section 6.3.3,
*Preprocessing:* As in Section 6.3.1.
*ADNP:* This is a variant of BVCR in which the *allDifferent* constraint is not propagated.[17] ADNP stands for *allDifferent not propagated*.

[17]ADNP uses a set *available* of values that are currently absent from single-valued domains. ADNP instantiates a variable $i$ to a value $u$ only if $u \in available$. When a variable $i$ is instantiated to a value $u$, then $u$ is removed from *available*, following Ullmann [1976]. Moreover, when a domain is reduced to a single value, v,

Table VII. Average Forward-Checking Search Times on *fapp*01-10

| fapp | time | to | $K$ |
|---|---|---|---|
| 01 | 18.73 | 4 | 11,163 |
| 02 | 5.20 | 8 | 14,005 |
| 03 | 9.71 | 3 | 22,734 |
| 04 | 3.72 | 8 | 28,876 |
| 05 | 108.76 | 6 | 34,655 |
| 06 | 0.78 | 7 | 34,166 |
| 07 | 101.72 | 3 | 24,998 |
| 08 | 0.01 | 8 | 27,992 |
| 09 | 186.14 | 7 | 18,795 |
| 10 | 5.22 | 5 | 40,803 |

$K$ is the average number of 1's in bit-matrices; higher $K$ signifies looser constraints.

Table VIII. Average Times for Finding All Subgraph Isomorphisms in 10,000 Trials with Duplicate Representation of Domains and with Only Bit-Vector Representation (BVO)

| | | | | | Duplicate | | BVO | |
|---|---|---|---|---|---|---|---|---|
| $n_\beta$ | $\rho$ | $\eta$ | directed | isos | av | sd | av | sd |
| 550 | 3 | 1 | no | 41,272.8 | 0.6776 | 0.0784 | 1.3267 | 0.1616 |
| 625 | 6 | 1 | no | 57,759.8 | 1.1025 | 0.1060 | 1.2193 | 0.1427 |
| 625 | 9 | 1 | no | 6.4 | 0.8873 | 0.0107 | 0.6801 | 0.0791 |
| 625 | 3 | 2 | no | 29,963.7 | 0.5616 | 0.0570 | 0.7015 | 0.0846 |
| 725 | 3 | 3 | no | 17.909.3 | 0.3292 | 0.0596 | 0.5619 | 0.0879 |
| 750 | 3 | 3 | no | 47.807.1 | 1.0445 | 0.0866 | 1.4307 | 0.1247 |
| 1000 | 3 | 4 | no | 16.691.4 | 0.4915 | 0.0515 | 0.6346 | 0.0622 |
| 575 | 3 | 1 | yes | 16,378.8 | 0.2701 | 0.0401 | 0.4066 | 0.0500 |
| 625 | 6 | 1 | yes | 255.9 | 0.0226 | 0.0002 | 0.0327 | 0.0003 |
| 675 | 6 | 1 | yes | 100,591.8 | 1.5456 | 0.1058 | 1.9650 | 0.2131 |
| 800 | 9 | 1 | yes | 69,377.0 | 1.1395 | 0.1650 | 1.3486 | 0.1984 |

In these experiments with graphs randomly generated as in Section 7.6.1, $n_\alpha = 500$, $\eta$ is the number of distinct vertex and edge labels, and the column headed *directed* indicates whether graphs are directed. The column headed *isos* shows average numbers of subgraph isomorphisms. Here, *sd* is the standard deviation of the average, not of the variate.

Duplicate (i.e., bit-vector and array) representation of domains is used because in Table VIII this is usually faster than representing domains only by bit-vectors. More importantly, duplicate representation allows incremental restoration, which enables experimentation on a larger scale than with pop-stack restoration. For this reason, incremental restoration is always used in Sections 7.4.1, 7.5, and 7.6. Pop-stack restoration would have been practicable in some cases, but switching between pop-stack and incremental restoration would have obscured the intercomparison of results.

### 7.4. Experiments with Graph Automorphism

*7.4.1. Random Graphs.* An *automorphism* is an isomorphism of a graph with itself. Although determination of automorphism of random graphs is nowadays a too-easy test of an isomorphism algorithm, Figure 17 shows some timings for comparison with [Foggia et al. 2001; Cordella et al. 2004]. Here, $G^\beta$ is the same graph as $G^\alpha$, which is connected and randomly generated except that no vertex has degree one, for reasons

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then v is removed from *available* unless v is already absent from *available*, in which case procedure *reduce* returns *consistent* = **false**. If, when at least one domain is multivalued, procedure *choose* finds no multivalued domain that includes at least one value in *available* then the effect is the same as when procedure *reduce* returns *consistent* = **false**. The set *available* is subject to pop-stack restoration.

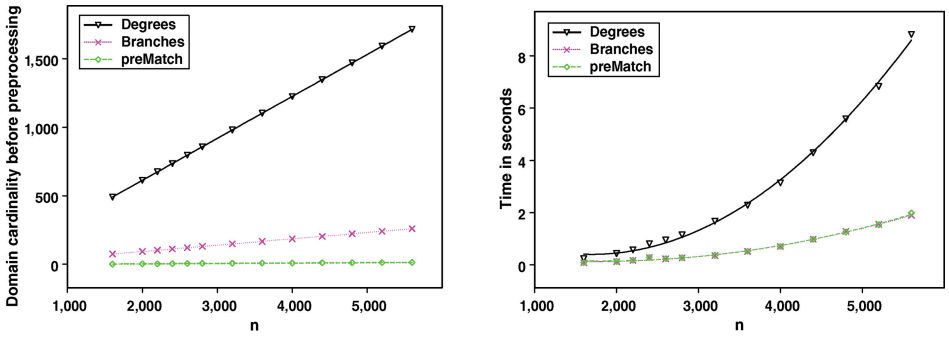



Fig. 17. Results of 100 trials, with algorithm BVCR with preprocessing and $\rho = 3$, which is the average degree. Here, $n$ is the number of vertices in the graph. (a) Average cardinality of domains before commencement of preprocessing. (b) Average time to find all automorphisms.

briefly indicated in Section 7.1.1. Figure 17 shows results obtained using three different vertex invariants

*degrees* a value $u$ is initially included in domain $D_i$ if $degreeOf(V_u^\beta) = degreeOf(V_i^\alpha)$.

*branches* a value $u$ is initially included in domain $D_i$ if the sum of degrees of vertices adjacent to $V_u^\beta$ equals the sum of degrees of vertices adjacent to $V_i^\alpha$. Results obtained using *branches* do not differ significantly from results obtained using distance-2-degrees instead of branches.

*prematches* a value $u$ is initially included in domain $D_i$ if $prematches(i, u)$ returns **true**, where *prematches* is as in Figure 8 except that the two instances of '>' are both changed to "$\neq$."

For each different number of vertices in Figure 17,

—the average number of automorphisms is less than 1.41;
—the average cardinality of domains after preprocessing is less than 1.0003;
—the average of the total number of elective instantiations during the search is less than 1.53.

This means that there is almost no search, and times in Figure 17(b) are almost entirely times taken by preprocessing. The curve-fit curves in Figure 17(a) are exactly linear; in (b) they are gently quadratic. Because there is almost no search, there is no point in comparing the performance of different search algorithms such as BVCR, forward checking and focus search on randomly generated graphs.

*7.4.2. Strongly Regular Graphs.* A graph $G = (V, E)$ that has $n$ vertices, all of these having the same degree $\rho$, is said to be *strongly regular* if there are integers $\lambda$ and $\nu$ such that

—every two adjacent vertices have $\lambda$ common neighbors, and
—every two nonadjacent vertices have $\nu$ common neighbors.

Finding automorphisms of strongly regular graphs can be a hard test for a vertex partitioning algorithm. In the present context, strongly regular graphs are of interest because preprocessing, as in Section 6.1, does not reduce any domain and is, therefore, useless; there is no point in comparing performance using unary constraints derived

Table IX. Details of 10 Sets of Strongly Regular Graphs

| Row | $n$ | $\rho$ | $\lambda$ | $\mu$ | nbGraphs | nbAutomorphisms |
|---|---|---|---|---|---|---|
| 1 | 25 | 8 | 3 | 2 | 1 | 28,800 |
| 2 | 25 | 12 | 5 | 6 | 15 | 52.27 |
| 3 | 26 | 10 | 3 | 4 | 10 | 18.9 |
| 4 | 27 | 10 | 1 | 5 | 1 | 51,840 |
| 5 | 28 | 12 | 6 | 4 | 4 | 10,290 |
| 6 | 29 | 14 | 6 | 7 | 41 | 11.85 |
| 7 | 35 | 16 | 6 | 8 | 3854 | 14.05 |
| 8 | 35 | 18 | 9 | 9 | 227 | 189.95 |
| 9 | 36 | 14 | 4 | 6 | 180 | 78.92 |
| 10 | 40 | 12 | 2 | 4 | 28 | 3,782.1 |

*nbGraphs* is the number of graphs in a set; *nbAutomorphisms* is the average number of automorphisms of graphs in this set.

Table X. Experimental results in row $x$ are obtained with the set of graphs in row $x$ of table IX.

| | BVCR | | BVFC | | Focus | |
|---|---|---|---|---|---|---|
| Row | time | nodes | time | nodes | time | nodes |
| 1 | 0.210 | 50,025 | 0.300 | 99,225 | 0.060 | 358,425 |
| 2 | 0.014 | 2,412 | 0.027 | 5,947 | 0.002 | 7,694 |
| 3 | 0.006 | 701 | 0.011 | 3,036 | 0.001 | 4,298 |
| 4 | 0.440 | 88,857 | 0.950 | 298,647 | 0.200 | 875,367 |
| 5 | 0.255 | 24,645 | 0.360 | 99,511 | 0.077 | 267,004 |
| 6 | 0.032 | 3,213 | 0.056 | 11,188 | 0.004 | 12,872 |
| 7 | 0.086 | 4,765 | 1.012 | 14,385 | 0.007 | 16,413 |
| 8 | 1.685 | 94,862 | 1.352 | 197,079 | 0.069 | 184,510 |
| 9 | 0.034 | 1,655 | 0.068 | 13,126 | 0.007 | 15,657 |
| 10 | 0.134 | 7,391 | 0.269 | 40,288 | 0.060 | 134,611 |

*time* is the average total time in seconds to find all automorphisms; *nodes* is the average number of search-tree nodes visited, which is the same thing as the average number of elective instantiations during the search. BVCR and BVFC here use pop-stack domain restoration.

from degrees or branches or prematching, because none of these reduce any domain. Every domain is initialized to contain exactly $n$ values.

Each row in Table IX provides information about one of 10 sets of strongly regular graphs obtained from http://cs.anu.edu.au/∼ bdm/data/graphs.html. Within a set, all the graphs belong to the same class, denoted by $srg(n, \rho, \lambda, \nu)$. Focus search is fastest in all rows in Table X, which shows timings. In Section 7.1, forward checking and focus search work best with high $\rho$. Forward checking is faster than BVCR only in Row 8 of Table X, where $\rho = 18$. In Row 8, the time taken by focus search is less than the time taken by BVCR by a factor of 24; this is the only row where the number of nodes visited by focus search is less than the number of nodes visited by forward checking. Although focus search visits the largest number of nodes in all other rows, it is fast because it does less work after each elective instantiation.

### 7.5. Experiments with Subgraph Isomorphism Benchmarks

Solnon [2010] has reported experimental comparison of recent subgraph isomorphism algorithms using benchmark pairs of graphs $(G^\alpha, G^\beta)$ available at http://www710.univ-lyon1.fr/∼csolnon/benchmarks.tgz. Timings in Table XI can be compared with Solnon's timings for other algorithms on the same benchmarks. Comparison is of course hazardous when algorithms are implemented in different programming languages by different programmers and when timings are obtained using different processors. It would be more meaningful to compare time-growth curves, as we have done for BVCR and

Table XI. Average Time in Seconds for BVCR, ADNP, BVFC and Focus Search on Benchmark Instances of Solnon [2010]

| Benchmark | $n_\beta$ | $\rho_\alpha$ | $\rho_\beta$ | BVCR | ADNP | BVFC | Focus |
|---|---|---|---|---|---|---|---|
| fixed | 200 | 5.67 | 6.00 | 0.050 | 0.047 | 0.008 | 0.130 |
| valence | 400 | 5.83 | 6.00 | 0.412 | 0.689 | 0.056 | 0.173 |
| | 800 | 5.91 | 6.00 | 4.795 | 8.603 | 0.390 | 1.723 |
| bounded | 200 | 4.12 | 5.98 | 0.002 | 0.002 | 0.002 | 0.005 |
| valence | 400 | 4.18 | 5.90 | 0.006 | 0.009 | 0.128 | 0.037 |
| | 800 | 4.27 | 5.99 | 0.026 | 0.036 | 0.105 | 0.045 |
| 4D | 256 | 4.11 | 6.04 | 0.030 | 0.044 | 0.026 | 0.016 |
| irregular | 625 | 4.28 | 6.23 | 0.083 | 0.267 | 1.104 | 0.133 |
| meshes | 1,296 | 4.36 | 6.35 | 2.699 | 3.521 | 2.566 | 6.028 |
| random | 200 | 2.82 | 4.45 | 0.018 | 0.037 | 0.022 | 0.096 |
| 0.01 | 400 | 4.03 | 8.18 | 10.000 | 10.450 | 63.291 | 4.010 |
| | 600 | 5.42 | 12.08 | 72.380 | 184.339 | 63.891 | 2.795 |
| random | 200 | 7.97 | 19.47 | 6.039 | 30.117 | 0.841 | 0.263 |
| 0.05 | 400 | 15.60 | 38.94 | - | - | 14.706 | 1.976 |
| | 600 | 23.41 | 58.43 | - | - | 89.447 | 10.333 |
| random | 200 | 15.08 | 37.85 | - | - | 8.862 | 1.435 |
| 0.10 | 400 | 25.17 | 50.55 | - | - | - | 89.278 |
| | 600 | 45.48 | 113.82 | - | - | - | 209.295 |
| scale | 200 | 5.43 | 6.03 | 0.015 | 0.018 | 0.016 | 0.017 |
| free | 600 | 5.43 | 6.02 | 0.268 | 0.268 | 0.267 | 0.238 |
| | 1,000 | 5.44 | 6.02 | 1.129 | 1.078 | 1.103 | 1.027 |

$\rho_\alpha$ and $\rho_\beta$ are average degrees of $G^\alpha$ and $G^\beta$; $n_\beta$ is the number of vertices in $G^\beta$. Each line in this table shows averages over 90 instances, except for the random instances, where averages are over 30 instances, and *scalefree*, where averages are over 20 instances. Moreover, each line shows average times for finding one isomorphism, except for the bottom three lines, which show average times for finding all isomorphisms. Algorithms are implemented in Modula-2. There are no timeouts except for two with focus search with *random* 0.10 and $n_\beta = 600$. A hyphen signifies that an algorithm is excessively slow.

focus search in Section 7.1.2, but appropriate time-growth curves have not yet been published for competitor algorithms.

In 20 trials with each of the *scalefree* benchmarks with $n_\beta = 200, 600, 1{,}000$, an isomorphism was found, respectively, in 9, 10, and 12 trials by preprocessing without any search. This is one reason why timings with these benchmarks are similar for the four algorithms. As in Section 7.1.2, focus search becomes more competitive the higher the average degree of $G^\alpha$. This is particularly clear with the random benchmarks.

ADNP is a variant of BVCR that was introduced in Section 7.3. Results for ADNP are included to help assess the extent to which propagation of the *allDifferent* constraint in BVCR is actually beneficial. In Table XI, the differences in times for BVCR and ADNP are not very significant, except where the average time for BVCR exceeds 2 seconds, but BVCR is very much faster than ADNP in Figure 18. Results of small-scale experimentation, as in Table XI, may be misleading.

### 7.6. Experiments with Subgraph Isomorphism of Randomly Generated Graphs

*7.6.1. Experimental Framework.* We aim to show how search time and number of isomorphisms depend on the sizes of the two graphs. We work with randomly generated graphs to facilitate systematic variation of problem parameters. Our procedure is as follows.

A graph $G^\beta$, having $n_\beta$ vertices, is generated randomly, except that no vertex has degree less than two. A subset of $n_\alpha$ vertices of $G^\beta$ are selected randomly to be the vertices of a new smaller graph $G^\alpha$. Every pair of these vertices that are adjacent in

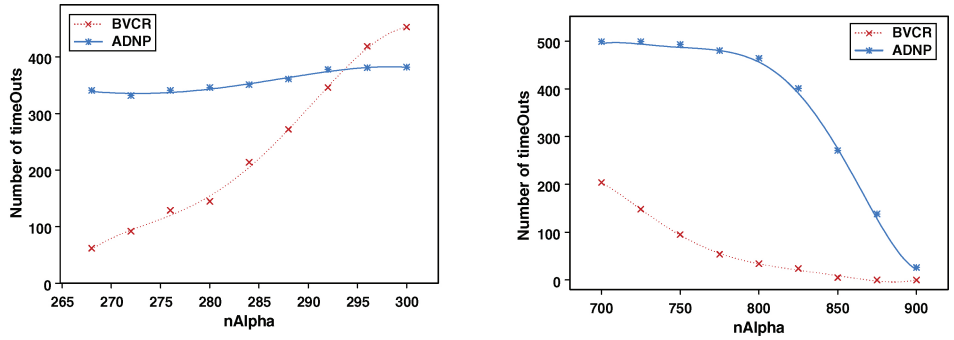



Fig. 18. The number of timeOuts when seeking *one* isomorphism in 500 trials with $n_\beta = 1{,}000$ and average degree $\rho = 3$. Here a *timeOut* is a trial in which the search is stopped at 10 seconds. (a) Tight side of maximum. (b) Loose side of maximum.

$G^\beta$ are also adjacent in $G^\alpha$. There are no other edges in $G^\alpha$, except that if $G^\alpha$ is found not to be connected, then, until $G^\alpha$ becomes connected, a succession of new edges are inserted into $G^\alpha$ and $G^\beta$ so as to preserve subgraph isomorphism. In most cases, very few new edges are inserted. In Section 7.6, $\rho$ denotes the average degree of graph $G^\beta$ before insertion of extra edges to ensure that $G^\alpha$ is connected.

In experiments with randomly generated labeled graphs, each vertex in $G^\beta$ is labeled with an ordinal chosen randomly within the range $1, \ldots, \eta$. Each edge in $G^\beta$ is also labeled with an ordinal chosen randomly within the same range. Of course, different ranges could be used for vertices and edges, but for simplicity we use equal ranges. Labels of vertices and edges in $G^\alpha$ are the same as those of the vertices and edges in $G^\beta$ to which they are mapped by the isomorphism inherent in the construction.

In all experiments reported in Section 7.6, the search is preceded by BVCR preprocessing, which is preceded by prematching. Prematching means applying unary constraints by invoking the appropriate version of *prematches*.

*7.6.2. Unlabelled Undirected Subgraph Isomorphism.* As before, $n_\alpha$ and $n_\beta$ are the numbers of vertices in graphs $G^\alpha$ and $G^\beta$, respectively. When $n_\beta = n_\alpha$, finding graph (not subgraph) isomorphism is not NP-Complete; instead, we have relatively gentle time growth, as in Figure 17(b). If we start with $n_\alpha$ much less than $n_\beta$ and increase $n_\alpha$ progressively until $n_\beta = n_\alpha$, the time to find one isomorphism at first increases exponentially, as in Section 7.1.2, and then decreases as we approach $n_\beta = n_\alpha$. The maximum in Figure 18 has not, so far as we know, been reported previously. Figure 18 also shows that ADNP, a variant of BVCR introduced in Section 7.3, is usually much slower than BVCR. This suggests that propagation of *allDifferent*, as in Section 6.3.1, substantially increases the speed of BVCR.

If we fix $n_\alpha$ and progressively increase $n_\beta$, starting near $n_\alpha = n_\beta$, the time to find one isomorphism at first increases exponentially, in Figure 19, until it reaches a further maximum, which again, so far as we know, has not been reported previously. When $n_\beta$ is increased beyond this maximum there are more edges in $G^\beta$ that could correspond to a given edge in $G^\alpha$. Because there are more solutions, finding one of these takes less time. Near the maximum the variance of timings is particularly high; the search is quick in most cases and very slow in others.[18] Despite the upward slope of the average-time plot

[18]Which is *heavy-tailed* behavior [Gomes et al. 2000; Hulubei and O'Sullivan 2006]. This also occurs at crossover in Section 7.1.2.

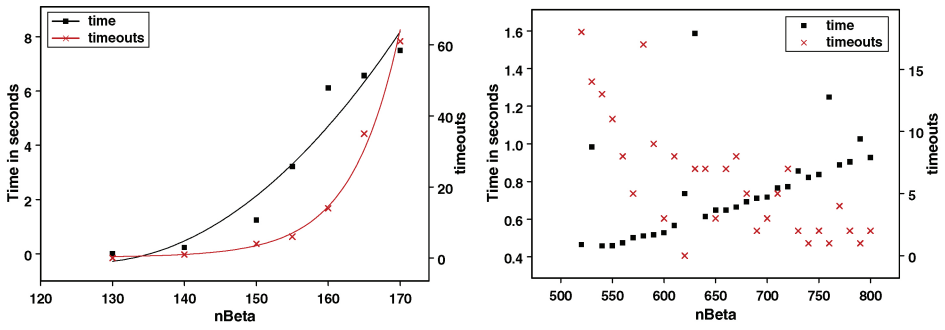



Fig. 19. Average time to find *one* isomorphism (lefthand axis) and number of timeouts (righthand axis) with BVCR, $n_\alpha = 100$, average degree $\rho = 3$, and 1,000 trials. Here, a *timeOut* is a trial in which the search is stopped at 1,000 seconds; *time* is the average over trials where there is no timeout. (a) Tight side of maximum. (b) Loose side of maximum.

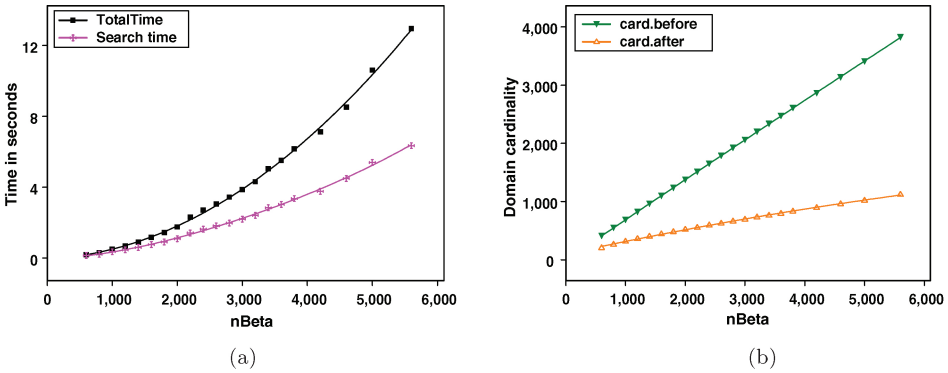



Fig. 20. Results of 1,000 trials with unlabeled directed subgraph isomorphism, BVCR, $n_\alpha = 100$, and average degree $\rho = 3$. (a) Average total time and search time to find *one* isomorphism. (b) Domain cardinalities before and after preprocessing.

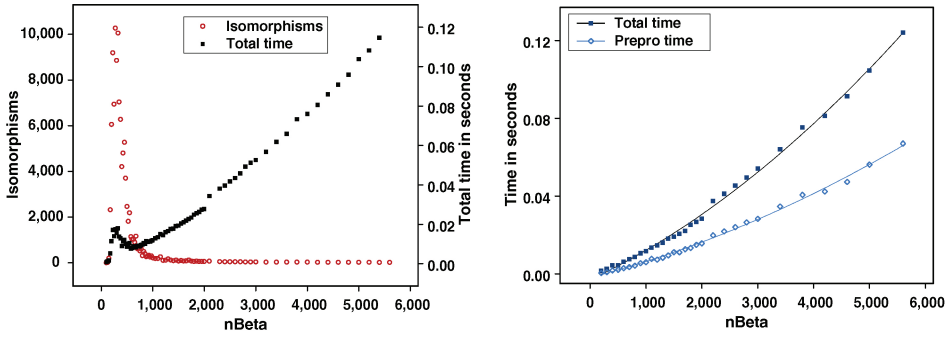
in Figure 19(b), the number of timeouts tends to decrease as $n_\beta$ increases. Moreover, the average time when $n_\beta > 150$ in Figure 19(a) exceeds all average times in Figure 19(b).

*7.6.3. Unlabeled Directed Subgraph Isomorphism.* With unlabeled directed graphs, and with the same parameters as in Figure 19, we see no maximum in Figure 20(a). The increasing difference between total time[19] and search time is almost entirely due to preprocessing, which removes an increasing number of values from domains, as can be seen in Figure 20(b).

*7.6.4. Labeled Undirected Subgraph Isomorphism.* When *all* isomorphisms are found, the sharp peak in Figure 21(a) is unexpected and unexplained. Again with the same parameters as in Figures 19 and 20, Figure 21(b) shows average total time to find one isomorphism. Most of this time is taken by preprocessing,[20] which is the same for Figures 21(a) and (b), and this is why the difference in total times is slight.

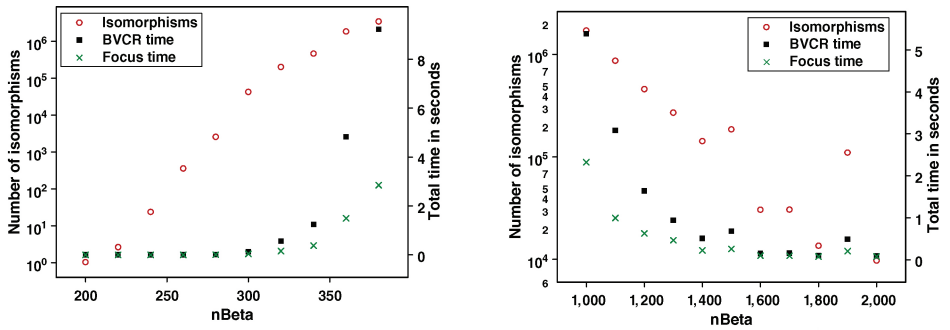
[19]In 1,000 trials there is exactly one timeout at 1,000 seconds when $n_\alpha = 1{,}000, 1{,}200, 1{,}400$ and this is not included in the average over the remaining 999 trials in Figure 20(a). There are no timeouts with other values of $n_\alpha$.

[20]When $n_\beta = 5{,}600$, the average cardinalities of domains before and after preprocessing are 653.2 and 1.632, respectively.




(a) (b)

Fig. 21. Results of 500 trials with labeled undirected subgraph isomorphism with BVCR, $n_\alpha = 100$, average degree $\rho = 3$, and with $\eta = 2$, which means that there are two possible labels for each vertex and for each edge. (a) Number of isomorphisms (lefthand axis) and total time to find all of them (righthand axis). (b) Average total time and preprocessing time to find only *one* isomorphism.



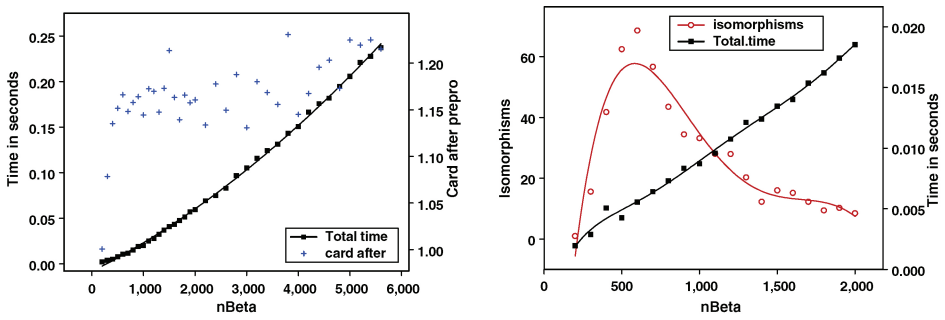

(a) (b)

Fig. 22. Five hundred trials with labeled undirected subgraph isomorphism, BVCR, and focus search, $n_\alpha = 200$, average degree $\rho = 3$ and $\eta = 2$ labels. The number of isomorphisms is plotted against the left axis, which is logarithmic. The total time, in seconds, to find all isomorphisms is plotted against the right axis, which is linear. (a) $n_\beta \leq 380$. (b) $n_\beta \geq 1{,}000$.

When we fix $n_\alpha = 200$ and increase $n_\beta$, the number of isomorphisms increases so rapidly that it is not practical to observe the top of the peak. Instead, Figure 22(a) shows the number of isomorphisms and the time to find all of them, up to $n_\beta = 380$. Figure 22(b) continues these results for $n_\beta \geq 1{,}000$. Focus search is competitive in these experiments because of the very low cardinality[21] of domains after preprocessing, as can be seen in Figure 23(a), righthand axis. We see no peak in total time to find one isomorphism, lefthand axis. When $\eta = 4$ and all isomorphisms are found, the peak is so small that we can see the whole of it in Figure 23(b).

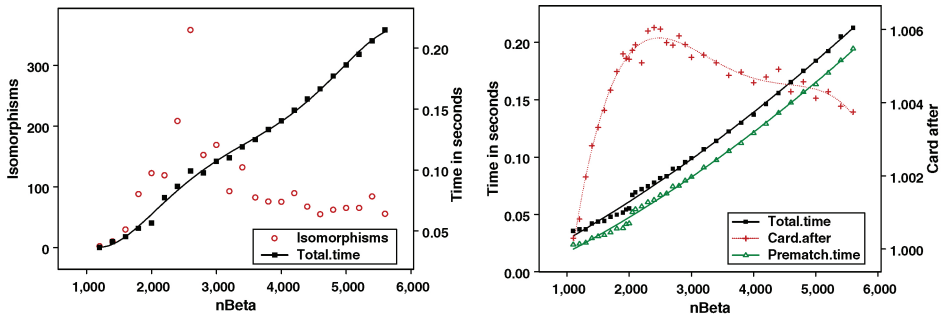
With $n_\alpha = 1{,}000$ and $\eta = 8$ labels, the slight peak in the number of isomorphisms in Figure 24(a) may perhaps be due to the slight peak in average domain cardinality after preprocessing. This cardinality, which is always less than 1.01, is plotted against the right hand axis in Figure 24(b). Total time to find all isomorphisms, in Figure 24(a), is

[21]Very low cardinality means that the amount of data moved by incremental restoration is exceptionally low, so incremental restoration is substantially faster than pop-stack restoration in this case, although in most other cases, incremental restoration is appreciably slower.




(a) (b)

Fig. 23. Labeled undirected subgraph isomorphism with BVCR, $n_\alpha = 200$, and average degree $\rho = 3$. (a) With $\eta = 2$ labels, 100 trials wherein the search stops as soon as the first isomorphism is found. (b) With $\eta = 4$ labels, 500 trials wherein all isomorphisms are found.




(a) (b)

Fig. 24. Results of trials with labeled undirected subgraph isomorphism with BVCR, $n_\alpha = 1{,}000$, average degree $\rho = 3$, and $\eta = 8$ labels. (a) Five hundred trials wherein all isomorphisms are found. (b) One hundred trials wherein the search stops as soon as the first isomorphism is found.

only very slightly greater than the time to find just one isomorphism in Figure 24(b). This is because when $n_\alpha = 1{,}000$ the total time is predominantly prematching time, as can be seen in Figure 24(b). Prematching checks $n_\alpha \times n_\beta$ possible correspondences, taking significant time when values of $n_\alpha$ and $n_\beta$ are high. The discontinuity in total-time curves at $n_\beta = 2,000$ is presumably due to the visible discontinuity in the prematching time curve, for which we have no explanation.

### 7.7. Molecular Graph Retrieval Experiments

The structural formula of a molecule can be regarded as a graph, in which vertices are labeled with atom-identifiers, such as “C”, “O”, “N”, and edges are labeled with bond-types,[22] which may be 1, 2, 3 or 4. In the following experiments, queries, and targets are graphs representing molecules; we seek all targets to which a query is exactly subgraph isomorphic. These experiments are intended to show how the effectiveness of trilabel matching, prematching, and preprocessing depend on the numbers of atoms in query and target molecules, using molecular data freely available to the

[22]Here, 4 denotes an aromatic bond as in a benzene ring. In all cases, we have converted 121212 benzene rings to 444444.

Table XII. Numbers of Atoms in Intervals 41 through 52

| Interval | Min number of atoms | Max number of atoms | Average number of atoms | Average number of bonds |
|---|---|---|---|---|
| 41 | 41 | 41 | 41.00 | 44.82 |
| 42 | 42 | 42 | 42.00 | 45.66 |
| 43 | 43 | 44 | 43.51 | 47.09 |
| 44 | 45 | 46 | 45.50 | 49.52 |
| 45 | 47 | 48 | 47.50 | 51.52 |
| 46 | 49 | 51 | 50.06 | 54.53 |
| 47 | 52 | 54 | 52.92 | 57.70 |
| 48 | 55 | 58 | 56.46 | 61.37 |
| 49 | 59 | 63 | 60.97 | 66.26 |
| 50 | 64 | 70 | 66.62 | 71.88 |
| 51 | 71 | 83 | 76.22 | 81.80 |
| 52 | 84 | 382 | 118.33 | 133.77 |

Within Interval 52, the number of atoms is distributed decreasingly across the range 84..382; the lower end of this range is very much more densely populated than the higher end.

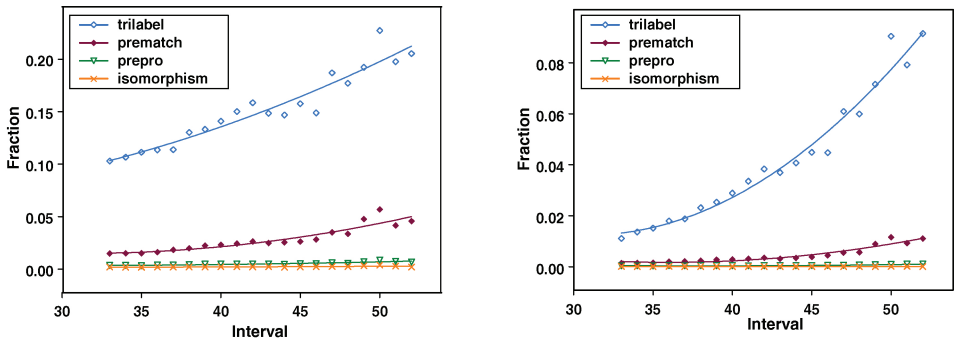



Fig. 25. Fraction admitted versus interval that contains target atoms. (a) Query has 12 atoms; $n_\alpha = 12$. (b) Query has 24 atoms; $n_\alpha = 24$.

public.[23] This data is of a kind for which there are well-established practical requirements for determination of subgraph isomorphism.

We have sorted this dataset into intervals, each containing at least 1,000 molecules. For $6 < n < 43$, every molecule in interval $n$ has exactly $n$ atoms. For $n > 41$, Table XII shows the range of numbers of atoms in molecules in interval $n$. Note that this range increases with $n$ and that interval 52 includes molecules containing up to 382 atoms. Molecules within each interval have not been sorted and remain in the same sequence as in the original dataset.

When comparing millions of pairs of molecular structures, we aim to spend minimal time using trilabels and prematching to rule out nonisomorphic comparisons. In Figure 25, which explores effectiveness of methods for *avoiding* search for isomorphism, $n_\alpha$ is the number of atoms in a query. These experiments use the first 3,000 molecules[24] having $n_\alpha$ atoms as queries, and use the first 1,000 molecules in each

[23]From the US Developmental Therapeutics Program via the bottom link on the page http://dtp.cancer.gov/docs/3d_database/Structural_information/structural_data.html.

[24]Excluding molecules that are not connected. A molecule is connected if and only if there is a path from any one of its atoms to all of its atoms via bonds. We also exclude any molecule that includes any atom other than “C”, “O”, “N”, “H”, “Cl”, or “S”, which occur most frequently in this dataset. Inclusion of unusual atoms would make a query too easy.

Table XIII. Average Time in Microseconds for Comparing One Query with One Target

| Number of atoms in query | BVCR | | | Focus | | |
|---|---|---|---|---|---|---|
| | Total time | Preprocess time | Search time | Total time | Preprocess time | Search time |
| 12 | 22.455 | 0.409 | 0.314 | 21.536 | 0.416 | 0.359 |
| 24 | 11.266 | 0.141 | 1.396 | 10.349 | 0.126 | 0.123 |

These averages are over the $3000 \times 20 \times 1000$ query-target comparisons in Figure 25. In these experiments, BVCR has pop-stack restoration.

interval 33 through 52 as targets. For 3,000 $\times$ 1,000 comparisons in each of these 20 intervals, Figure 25 shows four fractions of the 3 million comparisons

*trilabel* is the fraction wherein no trilabel occurs more times in the query than in the target.
*prematch* is the fraction wherein prematching leaves no domain empty.
*prepro* is the fraction wherein preprocessing leaves no domain empty.
*isomorphism* is the fraction wherein an isomorphism is found. The search terminates when an isomorphism is found.

Figure 25 shows that prematching greatly reduces the number of invocations of preprocessing, particularly when $n_\alpha = 24$. Although the number of invocations of prematching increases when *interval* increases, the number of invocations of preprocessing increases more slowly.

Table XIII shows the average total time, including disk access time, for comparing a query with a target. Cases where there is no preprocessing or no search[25] are included in average preprocessing and search times. For example, when there is no search, zero search time is included in the average search time. One reason why total time is less when $n_\alpha = 24$ is that trilabel and prematch filtering are more effective than when $n_\alpha = 12$, as can be seen in Figure 25. Although the search time for focus search is an order of magnitude less than for BVCR when $n_\alpha = 24$, there is not much difference in total time, because of the time taken by disk access, trilabel matching and prematching; also because search is avoided in many cases. The time growth curves in Figure 26 are not simply exponential[26]: Timings are similar for BVCR and focus search when $n_\alpha = 12$, but focus search is faster[27] when $n_\alpha = 24$.

Whereas Figure 25 plots fraction against target interval, Figure 27(a) plots fraction against the number, $n_\alpha$, of atoms in each query. Total time decreases as $n_\alpha$ increases because trilabel testing and prematching become more effective. Although focus search time decreases remarkably in Figure 27(d), the effect on total time is negligible.

Figures 25 and 27 show results of a four stage process: trilabel signature matching, prematching, preprocessing, and search. Preprocessing, as in Section 6.3.1, applies and propagates the *allDifferent* constraint, which is essential, but trilabel matching and prematching can be omitted. In Table XIV, which illustrates the effect such omissions, there are three cases.

(1) Trilabel matching and prematching are both applied.
(2) Trilabel matching is omitted and prematching is applied.

[25]For focus, the number of searches is exactly the same as it is for BVCR.
[26]Negative slope is attributable to decreasing cardinalities of domains.
[27]Low cardinality of domains improves the speed of focus search. For example, with $n_\alpha = 24$ there were 917 searches in interval 35; average domain cardinality and average search time were 5.465 and 305$\mu$secs, respectively. With $n_\alpha = 24$, there were 1,214 searches in interval 42; average domain cardinality and average search time were 5.100 and 131$\mu$secs, respectively.

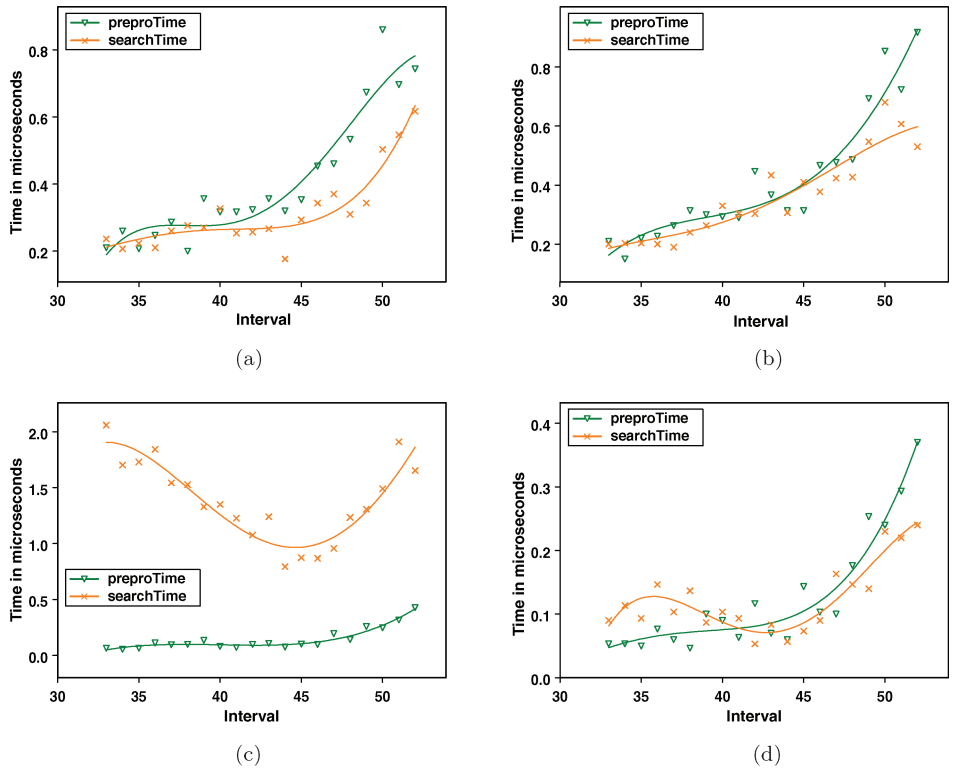



Fig. 26. Preprocess time and search time versus interval. (a) BVCR with $n_\alpha = 12$. (b) Focus search with $n_\alpha = 12$. (c) BVCR with $n_\alpha = 24$. (d) Focus search with $n_\alpha = 24$.

(3) Trilabel matching is applied and prematching is replaced by *hk*-attribute degree matching as in Section 6.6.

These results have been obtained with 60 queries,[28] which are not complete (hydrogen-suppressed) molecules, but instead are molecular substructures that are typical of practical queries. In these 60 queries, the minimum number of atoms is 5, the maximum number is 23, and the average is 10.82. Table XIV confirms that omission of stages increases average overall time. Comparing Case 1 with Case 3, we see that replacing prematching by *hk*-attribute degree doubles the total time.

## 8. CONCLUSION

Domain reduction is not an antidote for worst-case exponential time-complexity, but it does allow some real practical problems to be solved, for example, [Kohler et al. 2002; Chisholm and Motherwell 2004; Willett 2008; Bandyopadhyay et al. 2009; Hassan 2009]. For binary constraints, bit-vector domain reduction gains speed by using bit-parallel operations that are available in conventional processors. However, there may never be just one bit-vector domain reduction procedure that is always the best one to choose.

Incremental restoration allows us to solve bigger problems than pop-stack restoration, but is usually somewhat slower. Cumulative reduction is sometimes more than twice as fast as direct reduction, but is usually not much more than 30% faster.

[28]Kindly provided by Dr John Holliday, Department of Information Studies, The University of Sheffield, UK.

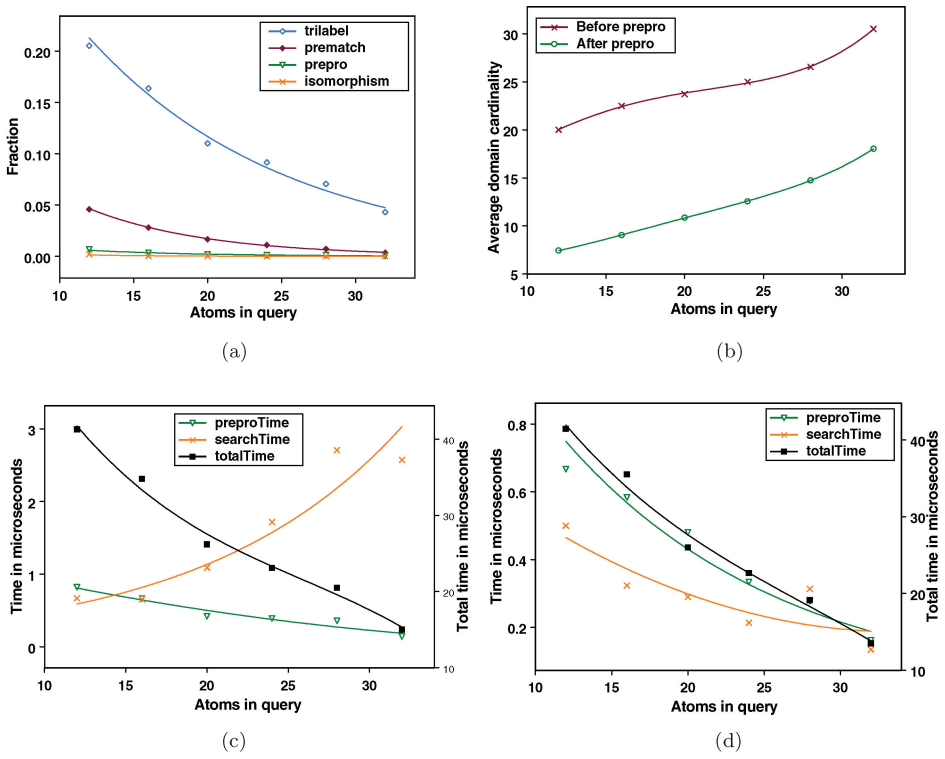



Fig. 27. Results of experiments with 1,000 target molecules in Interval 52 and 3,000 query molecules in Interval $n_\alpha$. The meaning of average times is the same as for Table XIII, except that these are averages over 3000 × 1,000 query-target comparisons. (a) Fraction admitted. (b) Average domain cardinality before and after preprocessing. (c) Average search time and preprocessing time (left axis) and total time (right axis) for BVCR. (d) Average search time and preprocessing time (left axis) and total time (right axis) for focus search.

Table XIV. Results of Comparison of 60 Queries with 1,000 Molecules in Interval 52

| Case | 1 | 2 | 3 |
|---|---|---|---|
| Number of prepros | 4,706 | 5,208 | 5,779 |
| Number of searches | 1,711 | 1,724 | 1,817 |
| Domain cardinality | 6.872 | 7.024 | 7.016 |
| Total time | 45.98 | 138.25 | 90.35 |

*Number of prepros* is the number of invocations of preprocessing within 60,000 query/target comparisons. *Domain cardinality* is the cardinality after preprocessing, averaged over the number of searches. *Total time* is the average in microseconds over 60,000 comparisons including cases where there is no prematch or no preprocessing or no search. The search algorithm is BVCR with pop-stack restoration.

Compared with direct reduction, cumulative reduction does not incur any additional memory cost, but it does make the reduction procedure rather more complicated.

There is a well-known trade-off between, on the one hand, light-weight domain reduction that requires many invocations because each achieves only a little reduction, and on the other hand, heavy-weight reduction that requires fewer invocations because each achieves more reduction [Bessière et al. 2002; Chmeiss and Saïs 2004]. Hitherto,

forward checking has been the usual example of a light-weight domain reduction procedure. The main original contribution of this article is the introduction of focus search, which is lighter-weight than forward checking. Focus search is an ultra light-weight process that does not have save/restore, nor dynamic variable ordering, nor does it update duplicate representations of domains during the search. Implementation of the *allDifferent* constraint is simpler in focus search than in forward checking.

Although heavy-weight reduction (e.g., BVCR) is fastest for many constraint satisfaction problems, light-weight reduction is sometimes an order of magnitude faster. Two examples are when the average degree of randomly generated constraint graphs is high (Figures 14(a), 15(c), 16(c)), and when constraint symmetry hampers domain reduction in the enumeration of automorphisms of strongly regular graphs (Table X). In these examples, forward checking is faster than BVCR, and focus search is even faster.

Besides introducing focus search, this article has also contributed an up-to-date algorithm for subgraph isomorphism, which differs from an earlier algorithm [Ullmann 1976] as follows.

(1) Straightforward implementation of a requirement that edges that correspond in an isomorphism must have matching labels.
(2) Dynamic variable ordering is applied with the weighting heuristic of Boussemart et al. [2004].
(3) Propagational domain reduction procedures employ a queue, following Mackworth [1977].
(4) Domain reduction is not applied to domains that are single-valued at the time of invocation of the domain reduction procedure. Linked lists serve to prevent the domain reduction procedure from visiting single-valued domains.
(5) The *allDifferent* constraint is applied within the domain reduction procedure. When a domain becomes single-valued, this value is removed from all other domains, and in this sense the *allDifferent* constraint is propagated, thus substantially reducing search time.
(6) Prematching is a nonpropagational domain reduction procedure that can be helpful before preprocessing.
(7) To avoid serial search for 1's in bit-vectors, domains can be represented by arrays as well as by bit-vectors, using Briggs-Torczon swapping to facilitate save/restore of array contents. An advantage of this duplicate representation is that it allows efficient incremental save/restore of domains when pop-stack restoration would require too much memory.

Technical developments reported in this article have allowed systematic experimentation on an unusually large scale, although it is only possible to explore an extremely small part of the multidimensional space of possible problems. With randomly generated binary constraint satisfaction (not isomorphism) problems, we have found that if the average degree $\rho$ is increased while other parameters are unchanged, the search becomes faster on the tight side of crossover but takes longer on the loose side because there are fewer solutions, so the average time to find one is greater. Between the two sides, there is a region where algorithms are intolerably slow. The size of this region increases when $\rho$ increases in Table IV.

For unlabeled undirected subgraph isomorphism there are *two* separate regions where search may be intolerably slow. As before, $n_\alpha$ and $n_\beta$ are the numbers of vertices in the smaller and in the larger graph, respectively. If $n_\beta$ is fixed while $n_\alpha$ increases, search time at first increases exponentially, and then decreases as $n_\alpha$ approaches $n_\beta$, in Figure 18, because graph (not subgraph) isomorphism is not NP-Complete. If $n_\alpha$ is fixed while $n_\beta$ is increased above $n_\alpha$, search time at first increases exponentially and

then decreases, in Figure 19, because there are more solutions. This second maximum is analogous to crossover.

NP-Completeness [Cook 1971] has hitherto discouraged development of algorithms for subgraph isomorphism. For directed unlabeled and undirected labeled subgraph isomorphism, which are the most important practical cases, our results suggest that average-time complexity is not exponential when $n_\beta < 5{,}600$. The time to find a single isomorphism increases quadratically with $n_\beta$ in Figures 20(a), 21(b), 23(a), and 24(b). It is, therefore, not surprising that algorithms for subgraph isomorphism have well-established practical applications in chemoinformatics.

Prematching is a valuable addition to the pre-existing armory of techniques for avoiding fruitless searches for molecular subgraph isomorphism. Searches are avoided more successfully as the molecular query size, $n_\alpha$, increases in Figures 25 and 27(a). This is why in Figures 27(c), 27(d) the total time per molecular comparison decreases as $n_\alpha$ increases, contradicting an assertion [Shang et al. 2008] that the larger the query graphs "the higher the cost for subgraph isomorphism testing."

We intend that future experimentation will include equitable comparison with Solnon's [2010] bipartite matching algorithm. We hope that future theoretical progress will explain peaks in numbers of isomorphisms in Figures 21(a), 22, 23(b), and 24(a).

## APPENDIX

## A. REPRESENTATION OF THE SET OF VARIABLES THAT HAVE MULTIVALUED DOMAINS

### A.1. Data Structure

While solving a constraint satisfaction problem, much time is usually spent within domain reduction procedures, which, therefore, require efficient access to adjacent variables whose domains are currently multivalued[29] without wasting time visiting other adjacent variables. To allow rapid access, we provide each variable with a doubly linked list of adjacent variables. This is doubly linked so that adjacent variables can easily be unlinked when their domains cease to be multivalued and can easily be relinked when multiple values have been restored to their domains.

More specifically, we provide a one-dimensional array of pointers, one for each variable. The pointer for $V_i$ points to a dummy record in a circular doubly linked list of multivalued variables adjacent to $V_i$. This list is circular and includes a dummy record to prevent the list from becoming empty, thus avoiding the need to check for this. These doubly linked lists are part of a multilist structure that is accessible via an index, which is another one-dimensional array of pointers, one for each variable, as in Figure 28. For a variable $V_i$, the element of the index points to a record for $V_i$ in the doubly linked list for an adjacent variable $V_j$. This record includes a pointer to the record for $V_i$ in the doubly linked list for another variable $V_k$ that is adjacent to $V_i$. This record includes a pointer to the record for $V_i$ in the doubly linked list for yet another variable $V_h$ that is adjacent to $V_i$, and so on, until all records for $V_i$ are included in the list pointed to by the index element for $V_i$. The index serves to identify records that should be unlinked/relinked from/into doubly linked lists, as will be explained.

In the doubly linked list of variables adjacent to $V_g$, the record for an adjacent variable $V_i$ includes three pointers

| | |
|---|---|
| *toNextAdjacent* | points to the next variable that is adjacent to $V_g$; |
| *toPreviousAdjacent* | points to the previous variable that is adjacent to $V_g$; |
| *toNextForSameVariable* | points to the record for $V_i$ within the doubly linked list for another variable that is adjacent to $V_i$ |

[29] In this section, *multivalued* means multivalued at the time of invocation of the domain reduction procedure.

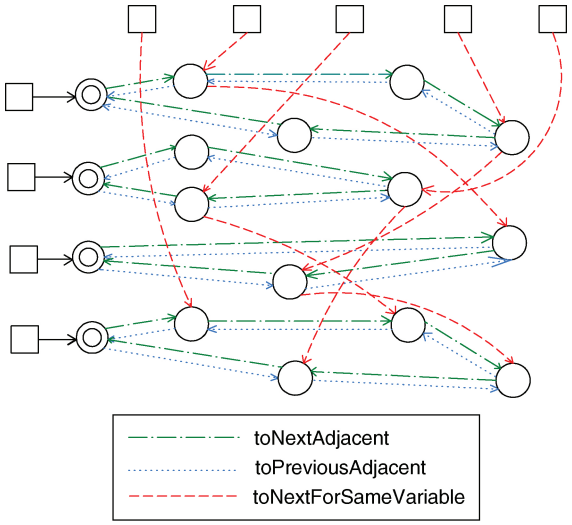



Fig. 28. An incomplete example of doubly linked circular lists threaded by index lists. At the top, rectangles in the horizontal row represent elements of the index. At the left, each rectangle corresponds to a variable and points to a circular list of adjacent variables. Concentric circles represent dummy records.

If the record for adjacent variable $V_i$ is the last in the list, then **toNextAdjacent** points to the dummy record for $V_g$. If the record for adjacent variable $V_i$ is the first in the list, then **toPreviousAdjacent** points to the dummy record for $V_g$. If $V_i$ is not adjacent to any further variable then its record has **toNextForSameVariable** = **nil**. As well as these three pointers, each record in a doubly linked list also includes a pointer to the relevant bit-matrix and, for adjacent variable $V_i$, the value of $i$.

During the search, when procedure *choose* finds that domain $D_i$ has become single-valued, records for $V_i$ in all doubly linked lists are located via the index and are unlinked. However, these records for $V_i$ remain linked into the list pointed to by the index element for $V_i$. When, because of backtrack, $D_i$ is no longer single-valued, then $V_i$ is relinked into the doubly linked lists for all variables adjacent to $V_i$. Relinking is achieved by updating pointers that point to the record for $V_i$. Pointers within this record remain unchanged because the sequence in which records are relinked is exactly the reverse of the sequence in which they were previously unlinked [Knuth 2000].

When used with direct or cumulative domain reduction, procedure *choose* selects, for elective instantiation, a variable whose domain is not already single-valued. We arrange that procedure *choose* proceeds

**for** each variable that has a multivalued domain **do** evaluate heuristic score ...

without visiting variables that have already been found to have single-valued domains. For this, we maintain an array *varSequence* so that elements *varSequence*[0], *varSequence*[1], ..., *varSequence*[*endSubscript*] identify variables that currently have multivalued domains and elements *varSequence*[*endSubscript*+1], ..., *varSequence*[$n-1$] identify variables that currently have single-valued domains. The main advantage of maintaining this array is that it readily shows which variables should be removed from, or inserted into, doubly linked lists.

Suppose, as a toy example, that there are only 10 variables, $V_0, \ldots, V_9$, and that before commencement of search, array *varSequence* is initialized to contain

$$\begin{array}{cccccccccc} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{array},$$

where the upper row of digits are array subscripts and the lower row are array elements that identify variables. If, for example, all variables are multivalued before procedure *choose* initially selects a variable $V_3$, then this procedure rearranges the array contents

$$\begin{array}{cccccccccc} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 0 & 1 & 2 & 9 & 4 & 5 & 6 & 7 & 8 & 3 \end{array}$$

and assigns *endSubscript*:= 8, signifying that variables identified by *varSequence*[0], . . . , *varSequence*[8] are multivalued. Domain $D_3$ will be made single-valued by elective instantiation; so, via the index, $V_3$ will be detached from the doubly linked lists associated with all variables that are adjacent to $V_3$.

Continuing this example, suppose that the next invocation of procedure *reduce* renders $D_1$ and $D_5$ single-valued and that procedure *choose* selects $V_2$ to be instantiated next. In this case, procedure *choose* swaps[30] the array contents

$$\begin{array}{cccccccccc} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 0 & 8 & 6 & 9 & 4 & 7 & 2 & 5 & 1 & 3 \end{array}$$

so that domains identified by *varSequence*[0], . . . , *varSequence*[*endSubscript*], where now *endSubscript* = 5, are multivalued. If the next invocation of the domain-reduction procedure does not yield an empty domain, then the next invocation of procedure *choose* will only process domains identified by *varSequence*[0], . . . ,*varSequence* [*endSubscript*], so some unnecessary work will be avoided. Far more importantly, variables identified by *varSequence*[*endSubscript* +1],. . ., *varSequence* [*previousEndSubscript*], where *previousEndSubscript* = 8, are detached from the doubly linked lists of adjacent variables.

Before updating *endSubscript*, procedure *choose* pushes onto a stack the value that *endSubscript* had at the time of this call of procedure *choose*. To illustrate the use of this, suppose now that in the last example shown, where finally *endSubscript* = 5, the next invocation of the domain reduction procedure does yield an empty domain, and that this is the case after each available value has been assigned to $V_2$ by elective instantiation. The search must now backtrack to the situation that existed just before $V_2$ was selected for instantiation. The assignment *endSubscript:= value popped off the stack*, which in this example means *endSubscript*:= 8, signifies that domains of variables *varSequence*[0], . . . , *varSequence*[*endSubscript*] are again multivalued. This efficient restoration does not put the contents of array *varSequence* back into their original sequence, but that does not matter for our purposes. What is again important is that variables identified by *varSequence*[6], . . . , *varSequence*[8] are relinked into doubly linked lists of adjacent variables.

### A.2. Implementation of Procedure *Choose*

Figure 29 shows the version of procedure *choose* that is used with bit-vector cumulative reduction (BVCR) and direct reduction (BVDR), which continue domain reduction until convergence. This procedure selects for elective instantiation a variable $V_i$ whose domain is not already single-valued due to implied instantiation. This procedure also identifies further domains that have become single valued, and decrements *endSubs* after swapping these out. The call *endPush(previousEndSubs)* at Line 22 simply pushes *previousEndSubs* onto a stack, which is named *endStack*. Although, for introductory simplicity, this is not shown, a call *relink(endSubscript)* at the end of Line 21 in Figure 1 achieves:

[30]This idea of swapping has come from Briggs and Torczon [1993] via Cheng and Yap [2008].

```
procedure choose(out i : integer; out terminal: boolean);
input (via global variables): cardinalities of domains;
output:  terminal = (all domains are single-valued);
        i such that V_i will be instantiated next (if terminal = false);
input and output: The following are accessed and updated via global variables:
        endSubcript; (* see Section A.1 *)
        varSequence, endStack;    (* of previous endSubscripts *)
        and doubly linked lists; (* see Section A.1 *)
begin
1    if endSubscript < 0 then (* all domains are single-valued *)
        terminal:= true; return
     end if;
2    min:= greatestAvailableValue; i := 0; j := 0; previousEndSubs:= endSubscript;
3    loop (* over variables already known to be multivalued *)
4       k := varSequence[j];
5       if D_k is now multivalued then (* V_k is a candidate for instantiation *)
6          compute heuristic score for the variable V_k;
7          if score < min then min:= score; i := k; iSubscript:= j end if;
8          if j = endSubscript then exit end if;
9          j := j + 1;
10      else (* swap k out of the range of multivalued variables in varSequence *)
11         varSequence[j]:= varSequence[endSubscript];
12         varSequence[endSubscript]:= k; endSubscript:= endSubscript - 1;
13         if j > endSubscript then exit end if;
14      end if;
15   end loop;
16   if endSubscript < 0 then (* no unlinking is required *)
        terminal:= true; endSubscript:= previousEndSubs; (* to prevent unlink/relink *)
        return
17   else terminal:= false
18   end if;
19   if iSubscript < endSubscript then (* swap i out of multivalued range *)
20      varSequence[iSubscript]:= varSequence[endSubscript]; varSequence[endSubscript]:= i;
21   end if; (* this swap is not required if iSubscript = endSubscript *)
22   endPush(previousEndSubs); (* to allow subsequent restoration *)
23   unlink(endSubscript, previousEndSubs); (* unlink V_i from lists identified by
           varSequence[endSubscript]..varSequence[previousEndSubs] *)
24   endSubscript:= endSubscript - 1; (* instantiation will make D_i single-valued *)
end choose;
```

Fig. 29. Procedure *choose* for use with BVDR and BVCR.

```
for i := endSubscript + 1 to value now at top of endStack do
   for V_j := each variable adjacent to V_i do
      re-link record for V_i into doubly linked list that is associated with V_j
   end for
end for
```

This call of *relink* is followed immediately by the call *endPop(endSubscript)*, which assigns to *endSubscript* the value popped off *endStack*.

With forward checking, we use a version of procedure *choose*, Figure 30, which may select for elective instantiation a variable whose domain is already single valued. Unlike domain reduction procedures that iterate until convergence, forward checking does not require efficient access to adjacent variables that had multivalued domains

```
procedure choose(out i: integer; out terminal: boolean);
input (via global variables): cardinalities of domains;
output:  terminal = (all domains are single-valued);
        i such that V_i will be instantiated next (if terminal = false);
input and output: The following are accessed and updated via global variables:
        endSubcript; (* see Section A.1 *)
        varSequence, endStack; (* of previous endSubscripts *)
        and doubly linked lists; (* see Section A.1 *)
begin
1   terminal:= true;
2   if endSubscript < 0 then return end if; (* all domains are single-valued *)
3   min:= greatestAvailableValue; i := 0; j := 0;
4   loop (* over variables that have not been electively instantiated *)
5     k := varSequence[j];
6     if D_k is multivalued then terminal:= false end if ;
7     compute heuristic score for the variable V_k;
8     if score < min then min:= score; i := k; iSubscript:= j end if;
9     if j = endSubscript then exit else j := j + 1 end if;
10  end loop;
11  if terminal then return end if;
12  if iSubscript < endSubscript then (* swap i out of multivalued range *)
13    varSequence[iSubscript]:= varSequence[endSubscript]; varSequence[endSubscript]:= i;
14  end if; (* this swap is not required if iSubscript = endSubscript *)
15  endPush(endSubscript); unlink(endSubscript, endSubscript);
16  endSubscript:= endSubscript - 1; (* instantiation will make D_i single-valued*)
end choose;
```

Fig. 30. Procedure *choose* for use with forward checking.

at the time of invocation of this procedure. Instead, it requires efficient access to all adjacent variables that are not already instantiated electively.

The loop at Lines 4 through 10 in Figure 30 does not swap out variables whose domains are found to be single-valued; such variables are candidates for elective instantiation. Therefore, the value of *endSubscript* is not changed by this loop. Records for the single selected variable are the only ones unlinked from doubly linked lists by the call of *unlink* at Line 15. These lists enable efficient access to all adjacent variables except those that have been instantiated electively.

## B. ARRAY REPRESENTATION OF DOMAINS

### B.1. Swapping in the Array Representation of Domains

Bitwise parallel **and** and **or** operations in Sections 3.2 and 3.3 necessarily work with bit-vector representation of domains. This representation does not allow efficient search for untried values in Figure 1, nor does it allow efficient enumeration of values within domain reduction procedures (Line 6 in Figures 2 and 3). As well as representing domain $D_i$ by a bit-vector $Dsets[i]$, we can also store values currently in $D_i$ in $Darrays[i, 1], \ldots, Darrays[i, Dcards[i]]$, where $Dcards[i]$ is the current cardinality of $D_i$. Values currently in $D_i$ can be enumerated simply by

**for** $k := 1$ **to** Dcards$[i]$ **do** nextValue:= Darrays$[i, k]$ ...

without searching for 1's in Dsets[i]. Following Briggs and Torczon [1993], as in Section A.1, a value $v$ can be removed from the *Darrays* representation of $D_i$ by swapping it out of the subarray $Darrays[i, 1], \ldots, Darrays[i, Dcards[i]]$. Values that are not

currently in domain $D_i$ reside in $Darrays[i,Dcards[i]+1], \ldots, Darrays[i,\delta]$, where $\delta$ is the greatest cardinality of any domain. Given the subscript that locates a value $v$ in $Darrays[i]$, value $v$ can be swapped out by

```
procedure swapOut(in i, subscript, v: integer; in out dCard: integer);
input: i identifies a domain; v is a value that is to be removed from D_i;
       subscript is such that v resides at Darrays[i, subscript];
input and output: dCard is the current cardinality of D_i;
       Darrays[1, 1]..Darrays[i, dCard] are the values currently in D_i;
begin
   Darrays[i, subscript]:= Darrays[i, dCard]; Darrays[i, dCard]:= v;
   dCard:= dCard−1
end swapOut
```

Values can be restored to the array representation of $D_i$ by appropriately incrementing $Dcards[i]$. As a toy example, in which the top row shows subscripts and the second row shows values in $Darrays[i]$,

$$\begin{array}{rrrrrrrrr} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 0 & 8 & 6 & 9 & 4 & 7 & 2 & 5 & 1, \end{array}$$

with $Dcards[i] = 4$, we have $D_i = \{0, 8, 6, 9\}$. Suppose for example that $\{4, 7, 2\}$ have been removed from $D_i$ by domain reduction. It is important that $\{4, 7, 2\}$ can be restored to domain $D_i$ simply by $Dcards[i] := Dcards[i] + 3$, without moving any value within $Darrays$. Values may not be restored into their original sequence within $Darrays$, but that does not matter here.

Many domains must be saved and restored during the search. Although this is not shown in Figure 1, the search routine saves the whole of the two-dimensional array $Darrays$ at Line 6 by pushing the whole of the one-dimensional array $Dcards$ onto a stack. It is important that the two-dimensional array $Darrays$ is not pushed onto a stack. At Lines 14, 18 and 21 in Figure 1, which does not show this detail, the two-dimensional array $Darrays$ is restored by popping the one-dimensional array $Dcards$ off the stack [Cheng and Yap 2008], without moving any value within $Darrays$.

Pop-stack save/restore of the entire array $Dsets$ can be avoided by using incremental restoration, which is easy when $Darrays$ and $Dcards$ are up to date and consistent with $Dsets$ at the time of restoration

```
oldCards:= Dcards; Dcards:= DcardStack[top]; top:= top - 1;
     (* Dcards has been popped off the stack *)
for i := 0 to n − 1 do (* for each variable *)
  for k := oldCards[i] + 1 to Dcards[i] do include Darrays[i, k] in Dsets[i]
  end for
end for
```

In many cases, we find experimentally that the use of double (i.e., $Dsets$ and $Darrays$) representation does not significantly improve the speed of search, and in some cases makes it slower. However, the availability of incremental restoration is a clear advantage of double representation.

### B.2. Direct and Cumulative Reduction with Array Representation

The direct reduction procedure in Figure 31 uses bit-vector and array representation of domains. After removing a value $u$ from $Dsets[i]$, this procedure swaps $u$ out of $Darrays[i]$ only if $D_i$ is not now empty. If $D_i$ would be emptied by removing the last value, this value is not removed from $Dsets$, nor is it swapped out of $Darrays$. In

```
procedure reduce(in h: integer; out consistent: boolean);
input:  h identifies the variable that has just been instantiated;
        Bit matrices are accessed via global variables;
input and output: Dsets is an array of bit-vectors representing domains;
        Dcards is an array of domain cardinalities;
        Darrays is an array of arrays that represent domains;
output: consistent = (no domain is empty);
begin
1   initialize queue to be empty; insert h into queue;
2   repeat
3     j:= variable removed from queue;
4     for each variable V_i that is adjacent to V_j such that D_i is multivalued do
        (* uSubscript is the subscript of the next value in Darrays[i] *)
5       uSubscript:= 1; dCard:= Dcards[i]; changed:= false;
6       while uSubscript ≤ dCard do (* for each value now in D_i do *)
7         u:= Darrays[i, uSubscript];
8         if M_j^i[u] * Dsets[j] = 0 then (* there is no support in D_j for u in D_i *)
9           if dCard = 1 then (* D_i would be empty after removing u *)
              w_ij:= w_ij + 1; consistent:= false; Dcards[i]:= 1; return
            end if;
10          remove u from Dsets[i]; changed:= true;
11          swapOut(i, uSubscript, u, dCard); (* swap u out of Darrays[i] *)
12        else uSubscript:= uSubscript + 1 (* to access next value in D_i *)
13        end if;
14      end while;
15      if changed and (i ∉ queue) then insert i into queue end if;
16      Dcards[i]:= dCard;
17    end for;
18  until queue is empty;
19  consistent:= true;
end reduce;
```

Fig. 31. A bit-vector direct reduction implementation of procedure *reduce* with array representation of domains.

this case, the assignment $Dcards[i]:= 1$ makes *Dsets*, *Darrays*, and *Dcards* mutually consistent, so incremental restoration can be used straightforwardly.

Array representation can also be used with cumulative reduction, as in Figure 32. Unlike direct reduction, cumulative reduction does not remove values from a domain $D_i$ sequentially, and, therefore, cannot update $Darrays[i]$ as soon as a value is removed. However, if $D_i$ is reduced, then $i$ is put into the queue, and will be $j$ in a subsequent iteration. After removing $j$ from the queue, cumulative reduction processes values in $D_j$ sequentially, aiming to reduce adjacent domains. During this sequential process for the first variable adjacent to $V_j$, the procedure updates $Darrays[j]$ and $Dcards[j]$.

The cumulative reduction procedure may return *consistent* = **false** when the queue contains variables for which *Darrays* is inconsistent with *Dsets*. This procedure does not waste time enforcing consistency that will anyway be overridden by pop-stack restoration. With pop-stack restoration, this is an advantage of cumulative reduction, but not with incremental restoration, which requires *Darrays*, *Dsets*, and *Dcards* to be mutually consistent. With incremental restoration, just before the cumulative reduction procedure returns *consistent* = **false**, we restore consistency by

```
for g:= each variable in the queue do
    for x := 1 to Dcards[g] do include Darrays[g, x] in Dsets[g] end for
end for
```

```
procedure reduce(in h: integer; out consistent: boolean);
input:  h identifies the variable that has just been instantiated;
        Bit matrices are accessed via global variables;
input and output: Dsets is an array of bit-vectors representing domains;
        Dcards is an array of domain cardinalities;
        Darrays is an array of arrays that represent domains;
output: consistent = (no domain is empty);
begin
1   initialize queue to be empty; insert h into queue;
2   repeat
3     j:= variable removed from queue; dCard:= Dcards[j];
4     if there is no variable adjacent to V_j that has a multivalued domain then
5       vSubscript:= 1;
6       while vSubscript ≤ dCard do (* without attempting domain reduction
          update Darrays[j] by removing values that are not in Dsets[j] *)
7         v:= Darrays[j, vSubscript];
8         if v in Dsets[j] then vSubscript:= vSubscript + 1 (* to access next v *)
9         else swapOut(j, vSubscript, v, dCard)
10        end if;
11      end while;
12    else
13      firstAdjacent:= true;
14      for each variable V_i that is adjacent to V_j such that D_i is multivalued do
15        B:= empty; vSubscript:= 1;
16        if firstAdjacent then (* update Darrays[j] and accumulate B *)
17          while vSubscript ≤ dCard do
18            v:= Darrays[j, vSubscript];
19            if v in Dsets[j] then B:= B + M_i^j[v]; vSubscript:= vSubscript + 1
20            else swapOut(j, vSubscript, v, dCard)
21            end if;
22          end while;
23          firstAdjacent:= false;
24        else (* Darrays[j] is up-to-date, so only accumulate B *)
25          while vSubscript ≤ dCard do
26            B:= B + M_i^j[Darrays[j, vSubscript]]; vSubscript:= vSubscript + 1
27          end while;
28        end if;
29        B:= Dsets[i] * B; (* B := {u ∈ D_i|u is supported in D_j } *)
30        if Dsets[i] ≠ B then (* D_i will be reduced *)
31          if B = 0 then w_ij:= w_ij + 1; consistent:= false; return end if
32          Dsets[i]:= B; (* reducing domain D_i *)
33          if (i ∉ queue) then insert i into queue end if;
34        end if;
35      end for;
36    end if;
37    Dcards[j]:= dCard;
38  until queue is empty;
39  consistent:= true;
end reduce
```

Fig. 32. A bit-vector cumulative reduction implementation of procedure *reduce* with array representation of domains.

With forward checking, *Dcards* is required for reference by procedure *choose*. The version of forward checking in Figure 33 counts 1's in bit-vectors while updating *Darrays* if *consistent* = **true**. If *consistent* = **false**, then, with pop-stack restoration, this procedure does not waste time updating *Darrays* and *Dcards*, which will be overwritten

```
procedure forwardCheck(in j, v : integer; in out Dsets: array of bit-vectors;
                                  out consistent: boolean);
input:  j identifies the variable that has just been instantiated;
        v is the value that has been assigned to j by elective instantiation;
        Bit matrices are accessed via global variables;
input and output: Dsets is an array of bit-vectors representing domains;
        Dcards is an array of domain cardinalities;
        Darrays is an array of arrays that represent domains;
output:  consistent = (no domain is empty);
begin
1   for each variable V_i adjacent to V_j that has not been electively instantiated do
2     Dsets[i]:= Dsets[i] * M_i^j[v];   (* D_i := D_i ∩ {u ∈ D_i | u is supported by v ∈ D_j} *)
3     if Dsets[i] = 0 then w_ij := w_ij + 1; consistent:= false; return end if;
4   end for
5   consistent:= true;
6   for each variable V_i adjacent to V_j that has not been electively instantiated do
        (* update Darrays and Dcards *)
7     uSubscript:= 1; dCard:= Dcards[i];
8     while uSubscript ≤ dCard do (* for each value in Darrays[i] *)
9       u := Darrays[i, uSubscript];
10      if u in Dsets[i] then uSubscript:= uSubscript + 1
11      else swapOut(i, uSubscript, u, dCard)
12      end if
13    end while;
14    Dcards[i]:= dCard;
15  end for
end forwardCheck;
```

Fig. 33. Forward checking with array representation of domains.

by restoration. With incremental restoration, if *consistent* = **false**, we make *Darrays* consistent with *Dsets* in the same way as for cumulative reduction. That is, we refer to *Darrays* to restore all values that have been removed from *Dsets*.

By referring to *Darrays*, the loop at Line 8 in Figure 33 avoids checking every bit in *Dsets*[$i$]. If we do not have duplicate representation of domains, we need to check every bit in *Dsets*[$i$] to update *Dcards*[$i$]. This is particularly unwelcome in forward checking, in which the domain reduction procedure is intended to be maximally simple. Another comment is that array representation enables the search routine to find untried values without visiting 0's in bit vectors. This is important for forward checking, which usually involves many more elective instantiations than direct or cumulative reduction.

### B.3. Enforcing the *AllDifferent* Constraint Using the Array Representation of Domains

With direct reduction we enforce *allDifferent* by inserting the fragment shown in Figure 34 between Lines 3 and 4 in Figure 31. This propagates the *allDifferent* constraint via the queue. Moreover, when a value is removed from a domain, *Dsets*, *Darrays*, and *Dcards* remain mutually consistent, so this fragment works correctly with pop-stack or incremental restoration.

When $j$ is removed from the queue during cumulative reduction, *Dcards*[$j$] is out of date. We, therefore, wait until *Dcards*[$j$] has been updated before checking whether *Dcards*[$j$] = 1. With pop-stack restoration, we can simply insert the fragment shown in Figure 34, with its Line 8 deleted, between Lines 37 and 38 in Figure 32. Line 8 is deleted because *Darrays*[$k$] will be updated when $k$ is removed from the queue.

With cumulative reduction and incremental restoration, if removing $u$ would empty $D_k$, then for each variable, $i$, in the queue, we insert into *Dsets*[$i$] all the values now

```
1   if Dcards[j] = 1 then (* D_j is single-valued *)
2     let u be the single value in D_j;
3     for each k such that D_k is multivalued do
4       if (k ≠ j) and (u ∈ Dsets[k]) then
5         if Dcards[k] = 1 then (* removing u would empty D_k *)
            consistent:= false; return
          end if;
6         remove u from Dsets[k]; Dcards[k]:= Dcards[k] - 1;
7         if k ∉ queue then insert k into queue end if;
          (* subsequently D_k may be found single-valued when k is removed from queue *)
8         find u in Darrays[k]; swap u out of Darrays[k];
9       end if
10    end for
11  end if
```

Fig. 34. Fragment inserted between Lines 3 and 4 in Figure 31 to enforce the *allDifferent* constraint when pop-stack or incremental domain restoration is used with direct reduction.

in $Darrays[i]$, to make these mutually consistent. This correction is a disadvantage of cumulative reduction.

With forward checking, Line 2 in Figure 33 becomes

$$\text{Dsets}[i]:= \text{Dsets}[i] * M_i^j[v] - \{v\},$$

so the value $v$ of $V_j$ is removed from domains of all uninstantiated variables that are adjacent to $V_j$. Furthermore, with pop-stack restoration, the amended forward-checking procedure ends by removing $v$ from all $D_k$ such that $k \neq j$, $V_k$ is not electively instantiated, and $V_k$ is not adjacent to $V_j$ (because adjacent domains have already been processed). If this empties $D_k$, then the procedure returns *consistent* = **false**. Otherwise, $v$ is found in, and swapped out of, $Darrays[k]$. As in the previous section, serial search for $v$ is unwelcome in forward checking, which is intended to be a quick-and-cheap procedure. With incremental restoration, further work is required, as before, to make *Dsets*, *Darrays*, and *Dcards* mutually consistent when the procedure returns *consistent* = **false**.

### C. RELATIONSHIP BETWEEN FOCUS SEARCH AND PARTITION SEARCH

This article is primarily concerned with constraints between pairs of variables. In problems where there are constraints between more than two variables, the constraints are said to be *nonbinary*. A set of variables that are together subject to a constraint constitute the *scope* of that constraint; the *arity* of the constraint is the number of variables in its scope.

Focus search belongs to a family of algorithms that also includes partition search for nonbinary constraint satisfaction [Ullmann 2007]. Like focus search, partition search employs a static instantiation sequence[31] and avoids save/restore. However, partition search uses a tabular representation of constraints: This means that the constraint on any given scope is represented by an explicit relational table of tuples. At the time when a set $Y_i$ of variables have already been instantiated, partition search works with a scope $S_j$ that maximally overlaps $Y_i$. Let $S_j^b$ be the set of variables in $S_j$ that are not in $Y_i$. Let $T_j^b$ be the set of tuples on $S_j^b$ such that each tuple in $T_j^b$ is part of a tuple on $S_j$

—that satisfies the constraint on $S_j$ and
—matches instantiated values of variables in $Y_i$ at this time.

[31]Also based on the maximum cardinality algorithm [Tarjan and Yannakakis 1984].

Partition search instantiates $S_j^b$ to successive tuples in $T_j^b$, which are obtained by accessing a data structure such as a hash table or a trie.

Now suppose that, at this same time, there is another scope $S_k$ that maximally overlaps $Y_i$, such that $S_k^b = S_j^b$. In this case, $S_j^b$ can in principle be instantiated to successive tuples in $T_j^b \cap T_k^b$, but if $|S_j^b| > 1$, then enumeration of this intersection would take an unwelcome amount of time. Actually partition search would successively instantiate $S_j^b$ to each tuple in $T_j^b$, and then check whether the instantiated tuple was also in $T_k^b$.

Again suppose that a set $Y_i$ of variables have already been instantiated, and now suppose also that every scope comprises exactly two variables. In this case, $T_j^b$ is a set of values of a single variable; this set can be represented by a bit-vector. An intersection such as $T_j^b \cap T_k^b$ is easily implemented by bitwise **and**. Focus search employs this intersection, whereas partition search does not, which is why partition search is useless with binary constraints. As explained previously, focus search accesses a bit-vector such as $M_j^i[u]$ in a one-dimensional array using subscript $u$. A one-dimensional array is inadequate when $|S_j \cap Y_i| > 1$.

Lines 1 through 4 of the focus search procedure *reduce* check the support of values in domains of variables that have not yet been instantiated. Partition search only checks consistency of values of instantiated variables.

Partition search takes account of the sequence of variables within each scope. To avoid the cost of constant redirection during the search, partition search renumbers the variables and also the scopes. Renumbering is unnecessary in focus search, which imposes the chosen static sequence via arrays *predecessor* and *successor*.

### D. TRILABEL SIGNATURE MATCHING

When a query graph is compared with hundreds of thousands of target graphs, the first step in each of these comparisons is an attempt to match the query graph trilabel signature with the target trilabel signature. The trilabel signature comparison process should be maximally efficient because it is usually executed a very large number of times. For each query trilabel, minimal time should be spent searching for a matching target trilabel.

Let $n_\lambda$ be the number of distinct vertex labels that may occur anywhere in the set of target graphs. We represent each distinct vertex label by a unique ordinal in the range $1, \ldots, n_\lambda$. These representative ordinals are chosen so that if vertex label $L_i$ is more frequent than vertex label $L_j$, then the ordinal that represents $L_i$ is greater than the ordinal that represents $L_j$. The frequency of a vertex label is proportional to the total number of its occurrences in the entire set of target graphs. We take the liberty of not distinguishing between a vertex label and the ordinal that represents it. Sorting vertex labels into increasing order means sorting vertex labels into increasing order of their representative ordinal.

Every trilabel is a triple $\langle$*vertexOneLabel, vertexTwoLabel, edgeLabel*$\rangle$ sorted so that *vertexOneLabel*$\leq$ *vertexTwoLabel*, which means that *vertexOneLabel* is not more frequent than *vertexTwoLabel*. We process trilabels in sequence of increasing frequency because failure is more likely earlier than later in this sequence. More specifically, trilabels are always processed in the lexicographic sequence illustrated in Table XV.

In the example in Table XV, as soon as *vertexOneLabels* are compared, we see that target trilabel $\langle 55, 65, 4\rangle$ does not match query trilabel $\langle 60, 62, 2\rangle$. Again, when the *vertexOneLabels* are compared we see that target trilabel $\langle 58, 60, 1\rangle$ does not match query trilabel $\langle 60, 62, 2\rangle$. After discovering this mismatch of *vertexOneLabels*, we *skip* futile comparisons between query trilabel $\langle 60, 62, 2\rangle$ and subsequent target trilabels

Table XV. Examples of Query and Target Trilabels

| Query | | | | Target | | | |
|---|---|---|---|---|---|---|---|
| First vertex | Second vertex | Edge label | Count | First vertex | Second vertex | Edge label | Count |
| 60 | 62 | 2 | 3 | 55 | 65 | 4 | 2 |
| 65 | 65 | 1 | 2 | 58 | 60 | 1 | 1 |
| | | | | 58 | 62 | 2 | 4 |
| | | | | 58 | 62 | 3 | 4 |
| | | | | 60 | 62 | 2 | 3 |
| | | | | 60 | 63 | 4 | 1 |
| | | | | 60 | 65 | 3 | 3 |
| | | | | 60 | 69 | 5 | 4 |
| | | | | 64 | 64 | 1 | 1 |
| | | | | 65 | 65 | 1 | 1 |
| | | | | 65 | 66 | 4 | 3 |
| | | | | 68 | 72 | 3 | 3 |

Table XVI. Head and Body of Target Signature

| Head | | - | Body | | |
|---|---|---|---|---|---|
| First vertex | nbOf trilabels | - - | Second vertex | Edge label | Count |
| 55 | 1 | - | 65 | 4 | 2 |
| 58 | 3 | - | 60 | 1 | 1 |
| 60 | 4 | - | 62 | 2 | 4 |
| 64 | 1 | - | 62 | 3 | 4 |
| 65 | 2 | - | 62 | 2 | 3 |
| 68 | 1 | - | 63 | 4 | 1 |
| | | - | 65 | 3 | 3 |
| | | - | 69 | 5 | 4 |
| | | - | 64 | 1 | 1 |
| | | - | 65 | 1 | 1 |
| | | - | 66 | 4 | 3 |
| | | - | 72 | 3 | 3 |

$\langle 58, 62, 2\rangle$ and $\langle 58, 62, 3\rangle$ that have $vertexOneLabel = 58$. Subsequently, after discovering the match between query trilabel $\langle 60, 62, 2\rangle$ and a target trilabel, we *skip* futile comparisons of query trilabel $\langle 65, 65, 1\rangle$ with further target trilabels that have $vertexOneLabel = 60$.

We skip futile comparisons by storing each signature in its own individual two-level structure that is similar to a de la Briandais [1959] trie. For each signature, the first level of the trie is the *head*, and the second level is the *body*. The head is an array of records that have two fields

—vertexOneLabel,
—the number of trilabels in this signature that have this vertexOneLabel for the first vertex.

The body is an array of records that have three fields

—vertexTwoLabel
—edgeLabel
—number of occurrences of this trilabel in this signature.

In the body there is one record corresponding 1:1 to each trilabel in the signature. For the query in Table XV, the head is

```
60  1
65  1
```

```
procedure signatureMatches(): boolean;
input: Query and target signatures in array-of-records form;
output: Return true iff every query trilabel matches a different target trilabel;
begin
1    targetHeadSubscript:= 1; targetBodySubscript:= 1; queryBodySubscript:= 1;
2    for queryHeadSubscript:= 1 to qNbFirstLabels do
3      with queryHead[queryHeadSubscript] do
4        qFirst:= firstVertexLabel; qNbTuples:= nbTuples;
5      end with;
6      queryBodyEndSubscript:= queryBodySubscript + qNbTuples;
7      loop (* seeking target firstVertexLabel = qFirst *)
8        if target[targetHeadSubscript].firstVertexLabel = qFirst then (* found *)
9          tNbTuples:= target[targetHeadSubscript].nbTuples;
10         if tNbTuples < qNbTuples then return false end if;
11         targetHeadSubscript:= targetHeadSubscript + 1; exit;
12       end if;
13       if (target[targetHeadSubscript].firstVertexLabel > qFirst) or
14         (targetHeadSubscript = tNbFirstLabels) then return false
15       else
16         targetBodySubscript:= targetBodySubscript + tNbTuples;
17         targetHeadSubscript:= targetHeadSubscript + 1
18       end if
19     end loop;
20     loop (* for each entry in query body that has this qFirst *)
21       with queryBody[queryBodySubscript] do
22         qSecond:= secondVertexLabel; qEdge:= edgeLabel; qCount:= count;
23       end with;
24       loop (* seek matching entry in target body *)
25         with targetBody[targetBodySubscript] do
26           tSecond:= secondVertexLabel; tEdge:= edgeLabel; tCount:= count;
27         end with;
28         if tSecond > qSecond then return false end if;
29         if (tSecond < qSecond) or (tEdge < qEdge) then
30           if tNbTuples = 1 then return false (* because no more tSeconds for tFirst *)
31           else tNbTuples:= tNbTuples - 1; targetBodySubscript:= targetBodySubscript + 1;
32           end if
33         elsif (tEdge > qEdge) or (qCount > tCount) then return false
34         else (* match has been found in target body *)
35           targetBodySubscript:= targetBodySubscript + 1;
36           tNbTuples:= tNbTuples - 1; exit
37         end if;
38       end loop; (*loop over target body *)
39       queryBodySubscript:= queryBodySubscript + 1;
40       if queryBodySubscript = queryBodyEndSubscript then exit end if;
41       if tNbTuples = 0 then return false end if;
42     end loop;
43     targetBodySubscript:= targetBodySubscript + tNbTuples;
44   end for; (* for query head subscript *)
45   return true
end signatureMatches
```

Fig. 35. Transcription of a signature matching procedure.

and the body is

```
62  2  3
65  1  2
```

The number 3 at the right end of the first line in the body signifies that the trilabel $\langle 60, 62, 2\rangle$ occurs three times in the query graph. Similarly, the number 2 in the next line signifies that the trilabel $\langle 65, 65, 1\rangle$ occurs twice in the query graph. Table XVI shows the head and body of the target signature in Table XV.

Figure 35 is a transcription of our signature matching procedure. For our example, this procedure visits the first three records in the target head, seeking *firstVertex Label* $= 60$. The procedure skips the first four records in the target body because these are associated with *firstVertexLabel* $< 60$. After finding the matching trilabel $\langle 60, 62, 2\rangle$, the procedure visits the next two records in the target head, seeking *firstVertexLabel* $=$ 65, and skips four records in the target body that are associated with *firstVertexLabel* $< 65$. The procedure terminates as soon as it finds the matching trilabel $\langle 65, 65, 1\rangle$.

If the example is amended so that the first query trilabel is now $\langle 54, 62, 2\rangle$, the first iteration of the loop at Lines 7 through 19 returns **false** at Line 14 in Figure 35, when no body records have been visited. If, instead, the first query trilabel is now changed to $\langle 56, 62, 2\rangle$, the second iteration of the loop at Lines 7 through 19 returns **false** at Line 14, when no body records have been visited. If, instead, the first query trilabel is changed to $\langle 60, 61, 2\rangle$, the procedure returns **false** at Line 28 when just one query body record and one target body record have been visited. For signatures that do not match, the procedure is intended to return **false** as soon as possible. For our initial example where the query signature is $(\langle 60, 62, 2\rangle, \langle 65, 65, 1\rangle)$, the procedure returns **true** without visiting the last two target trilabels.

Hundreds of thousands of target signatures cannot all reside in fast memory. Reading successive target signatures in turn individually from disk would take too long because of latency. Instead, we store target signatures on disk within big pages, each holding many target signatures. We ensure that each target signature is wholly within a single page. Here a page is a fixed-size block of, for example, 20,000 bytes. When a page is read from a disk, it looks like an array of bytes. We do not copy successive target signatures from this into the array-of-records structure described earlier. Instead, our signature matching procedure works with target signatures directly in array-of-bytes form in the page buffer, to save time. Figure 35 is a transcription in the sense that it has the target signature in array-of-records form, because this is easier to understand. This procedure does, however, work with the query signature in array-of-records form.

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