Modelling Languages, Model Expansion, and MXG

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Outline

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Combinatorial Search Problems

Occur Widely in Applications:

- Operations: Timetabling, Scheduling, Planning, Routing, ...
- HW/SW: Equivalence, Verification (bug finding), test generation ...
- Bioinformatics: phylogeny, haplotyping, protein folding, ...
- ...

Many are hard - solving is expensive:

- NP-hard, and hard in practice
- good application-specific implementations expensive

Solve by reduction

E.g., Solve NP-search problems by reduction to SAT (say)

SAT Solving: Good News

SAT solver technology is effective for a growing collection of problems

SAT Solving Methodology

1. Design a reduction from given problem to SAT
2. Implement reduction (say with a C program)
3. Run off-the-shelf SAT solver(s)

Plenty more to do, but "Ground Solver" work mature and healthy:

- theory (proof complexty, tractable cases, etc.)
- impressive implementations (SAT, SMT, CSP, ASP, etc.)
- experimentation
- application successes
- steady progress

SAT Solving: Bad News

Refinement of reductions is needed in practice:

- multiple iterations of 2 and 3
- time-consuming, error-prone process
- for specialists

"Front-End" tools would be useful

- modelling languages – to model *problems*
- automatic reduction to SAT – i.e., grounding
- debugging aids
- ...

Modelling Languages

Solvers could be exploited more fully with "front end" modelling languages

Alternate Methodology

1. Construct a Declarative Problem Model
2. Grounder produces SAT instance from Model and Instance
3. Run SAT solver

- speed up development time;
- facilitate more experimentation;
- reduce errors
- improve performance (?!)

Example: Social Golfer Problem

Given $g \times s$ golfers and w weeks,
find a schedule for golfers to play:

- w games
- in s groups of size g
- such that not two golfers play together twice.

Social Golfer Problem in Essence

```
given    w,g,s:int ( 1..  )
letting  golfers be new type of size g × s
find     schedule:set (size w)
            of partition (numParts g, partSize s) from golfers
such that
         ∀ week1, week2 ∈ sched . week1 != week2 →
            ∀ group1 ∈parts(week1), group2 ∈parts(week2) .
               |group1 ∩ group2| < 2
```

Example: Social Golfer Problem, cont'd

Social Golfer Problem in ESRA

cst weeks, groups, groupsize : N

dom$Players = 1..groups \times groupsize$,

$Weeks = 1..weeks$, $Groups = 1..groups$;

var $Sched : (Players \times Weeks) \rightarrow^{groupsize \times weeks} Groups$

solve

$\forall(h : Groups, w : Weeks)count(groupsize)(p : Players | Sched(p, w) = h) \wedge$

$\forall(p1 < p2 : Players)count(0...1)(w : Weeks | Sched(p1, w) = Sched(p2, w))$

Social Golfer Problem in NP-Spec

SPECIFICATION

IntFunc({1..groups×groupsize} >< {weeks}, Schedule, 1..groups).

fail ← COUNT(Schedule(*,W,Gr),X), X != groupsize.

fail ← Schedule(P1,W1,Gr1), Schedule(P2,W1,Gr1), P1 != P2,
Schedule(P1,W2,Gr2), Schedule(P2,W2,Gr2), W1 != W2.

Modelling Languages: Bad News

Recognized need $\Rightarrow$ many projects:

- "Constraint Modelling" languages: Essence, ESRA, OPL, ...
- Answer Set Programming languages: DLV, Lparse, ...
- FO(ID)-based languages: MXG, IDP,
- NP-Spec & Spec2SAT, ASPPS, ...

But rather ad hoc: Modelling language work relatively immature.

As a field:

- little or no theory,
- little analysis or careful experimentation
- few tools and techniques
- few good implementations
- few applications

Yet many hard problems.

Outline

Formal Foundation: Model Expansion

Claim: we should start with a formal foundation

Model Expansion for Logic $\mathcal{L}$ ($\mathcal{L}$-MX)

`Given:`

- finite σ-structure $\mathcal{A} = (A; \sigma^{\mathfrak{A}})$,
- formula ϕ of logic $\mathcal{L}$, with vocabulary $\sigma \cup \varepsilon$

`Find:`

- $\sigma \cup \varepsilon$-structure $\mathcal{B} = (A; \sigma^{\mathfrak{A}}, \varepsilon^{\mathfrak{B}})$, s.t. $\mathfrak{B} \models \phi$
  (i.e., An expansion of $\mathcal{A}$ that satisfies ϕ)

- Expansion of a structure a standard notion in model theory
- MX as as a task proposed in (M.-Ternovska'05) as formal basis for declarative programming for search problems:
  - Problem instance: finite structure $\mathcal{A}$,
  - Formula ϕ specifies relation between instances and solutions,

MX and Declarative Programming

Graph Colouring as FO-MX

- Instance: Graph $\mathcal{A} = G = (Vtx \cup Clr; Edge^G)$,
- Expansion Vocabulary: $Colour$ (where $Colour : Vtx \longrightarrow Clr$).
- Problem specification:
$$\phi = \forall x \forall y (Edge(x, y) \supset Colour(x) \neq Colour(y))$$
- Solutions: Interpretations for $Colour$ such that
$$\mathcal{B} = (Vtx \cup Clr; Edge^G, Colour^B) \models \phi$$

- ϕ is a problem specification.
- $\mathcal{L}$ can be tailored to:
  - what problems we want to express;
  - natural ways to express problems of interest.
- Every computational search problem can be formalized as MX, (for suitable $\mathcal{L}$).
- Most existing languages naturally viewed as MX-specifications.

Descriptive Complexity Theory

Characterizes complexity classes in terms of logics:

- NP = $\exists SO$-definable finite structures (Fagin'74)
- PH = SO-definable finite structures
- P = LFP-definable ordered finite structures (Immerman-Vardi)

Suggests logics as declarative programming languages for complexity classes

- FO-MX captures NP
- Conventional Wisdom: not practically useful
- We strongly disagree
- Constraint Modelling languages are doing it
  although many authors don't know it
- E.g., languages describe MX tasks in (syntactic variants of extensions of) standard logics. *(***M***–Ternovska '08 examines ESSENCE)*,

Two Questions

Why "FO-MX" not ∃SO?

- emphasize we must witness the SO variables
- we are interested in MX for various logics: e.g.,
  - GF_k(ID)-MX
  - Π_2(ID)-MX

Why do we care about "capturing" complexity classes?

- provide assurance the user can model their problem
- provide assurance of "implementability", e.g.:
  - we want polytime grounding for problems in NP;
  - the above languages do not provide it!

Outline

The MX Project

- Joint work with E. Ternovska, plus students, post-docs and others
- Main Goal: Build practical MX-based tools for solving search problems.

Project tennets:

- Logic from top to bottom

  Classical logic, as far as possible

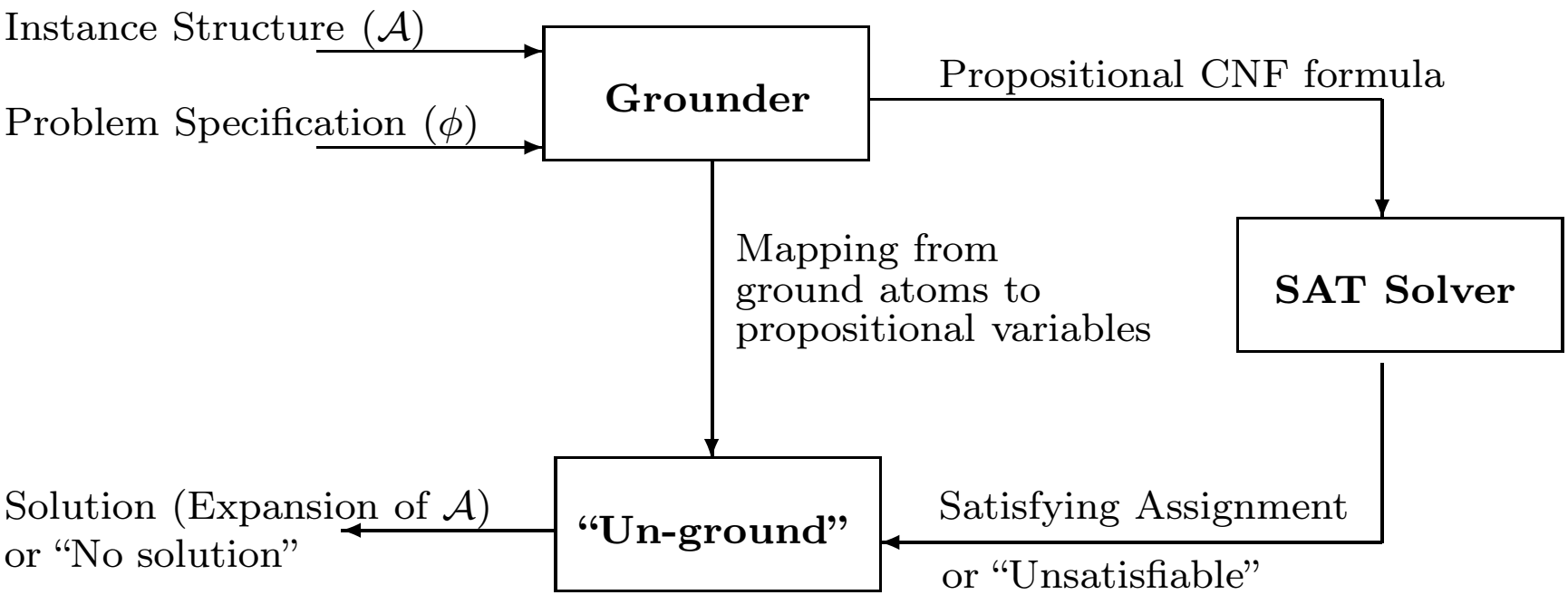
- Every component based on theory

  no implementation without formalization

- Theory and Practice proceed hand-in-hand

- Active development of theory under way,
- Prototype Solver MXG, for solving NP-search by reduction to SAT.

MXG General Solving Scheme



MXG: Modelling Language

- Classical First Order Logic, without functions

$$\textit{FO-MX} \equiv \exists \textit{SO} \Rightarrow \textit{Captures NP (Fagin'74)}$$

- Extend with:
  - Sorts : (rudimentary type system)
  - Order : All structures are ordered.
    - ★ $<, \leq, \ldots, \forall x < y$, MIN, MAX, SUCC, for each sort.
  - Inductive Definitions: FO(ID)-MX
  - Cardinality Constraints :
    - ★ e.g. $\forall u : \mathit{CARD}(1; v; \mathit{Edge}(v, u))$ = "each vertex has in-degree 1".
- Future:
  - Functions
  - Arithmetic
  - Further Aggregates
  - Type System
  - Syntactic Variants: e.g., Extended SQL

Example

MXG Specification for Graph Colouring

```
Given:
    type Vertex Colours;
    Edge( Vertex, Vertex )

Find:
    Colour( Vertex, Colours )

Satisfying :
    ∀ x y z>y : ¬ ( Colour(x,y) ∧ Colour(x,z) )
    ∀ x y : Edge(x,y) ⇒ (∀ z: ¬ (Colour(x,z) ∧ Colour(y,z)))
    ∀ x: ∃ z : Colour(x,z)
```

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Grounding for MX

Grounding is an important system component, but:

- Most grounders do (nearly) naive substitution for variables.
- no theory to support serious study or development of techniques

Grounding as Generalized Query Answering

- Boolean Query: $\phi : \mathcal{A} \rightarrow \{true, false\}$
- MX Specification: $\phi : \mathcal{A} \rightarrow \{$ expansions satisfying $\phi\}$
- MX Grounding: $\phi : \mathcal{A} \rightarrow \psi$: Mod($\psi$)=$\{$ expansions satisfying $\phi\}$

- Reduced grounding for a sentence ϕ wrt structure $\mathcal{A}$ is:
  - a ground formula ψ,
  - no instance vocabulary symbols (from $\mathcal{A}$),
  - any expansion of $\mathcal{A}$ satisfies ϕ, iff it satisfies ψ.
- MXG: constructs reduced grounding using generalized relational algebra [Patterson et al 2007].
- Now: use database techniques, etc., to improve performance.

Outline

Performance Comparison: MXG *vs.* ASP Solvers

Specification for Latin Square Compl.

```
Given:    type Num;
          Preassigned(Num, Num, Num)

Find:     Cell(Num, Num, Num)

Satisfying :
        ∀ x y z : (Preassigned(x, y, z) ⊃ Cell(x, y, z))
        ∀ x y : CARD(1, z; Cell(x, y, z))
        ∀ x z : CARD(1, y; Cell(x, y, z))
        ∀ z y : CARD(1, x; Cell(x, y, z))
```

Key

MXG+MXC

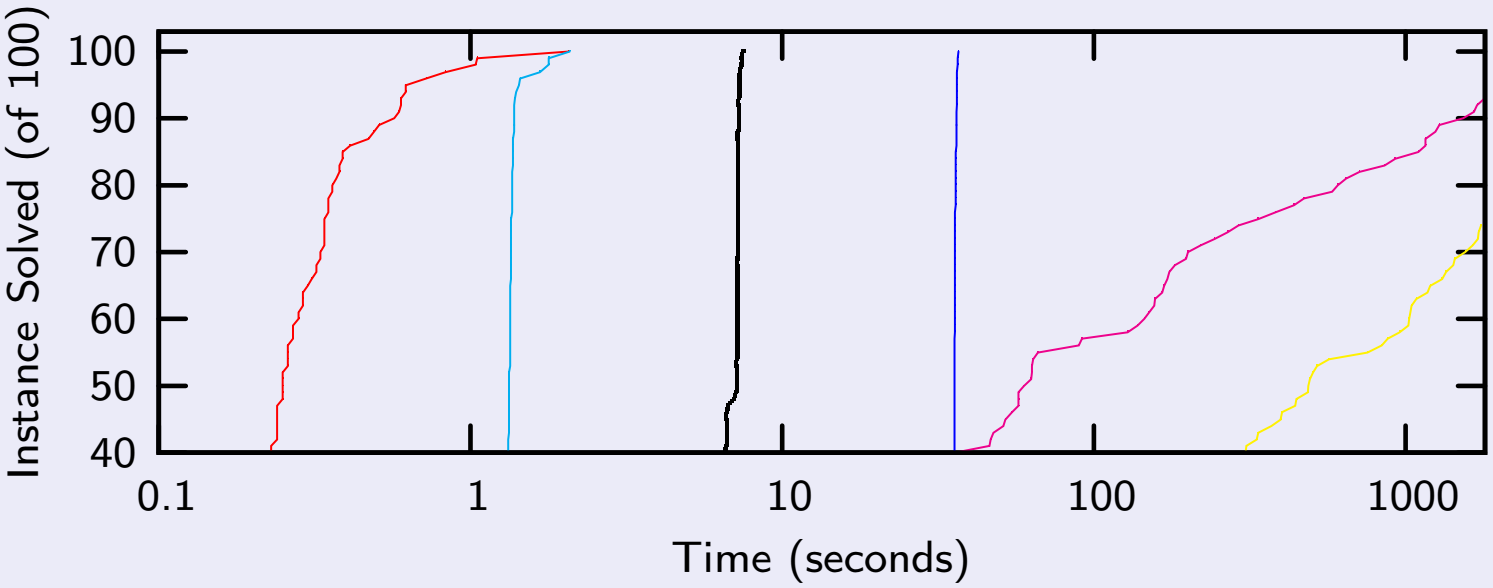
clasp

DLV

Smodels

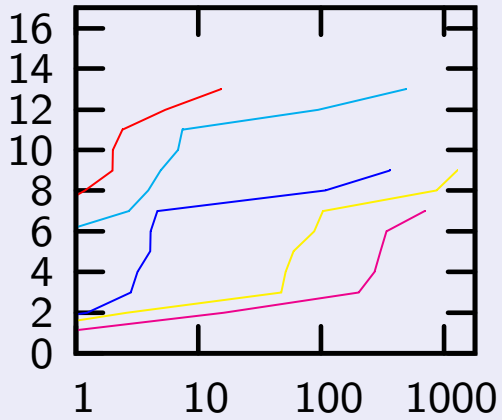
MidL

Plot

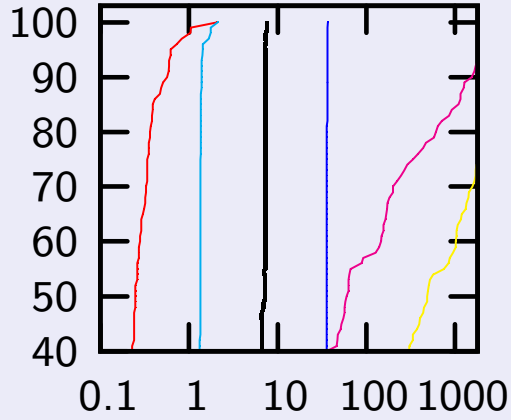


MXG Performance

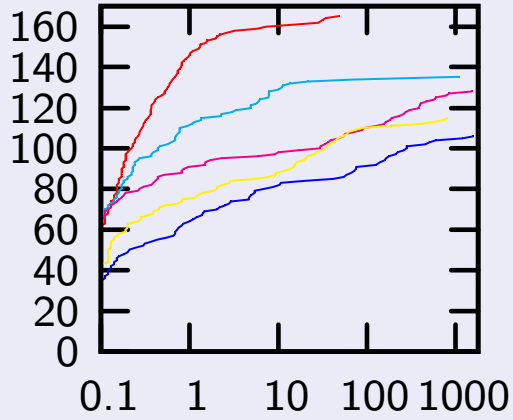
K-Coloring



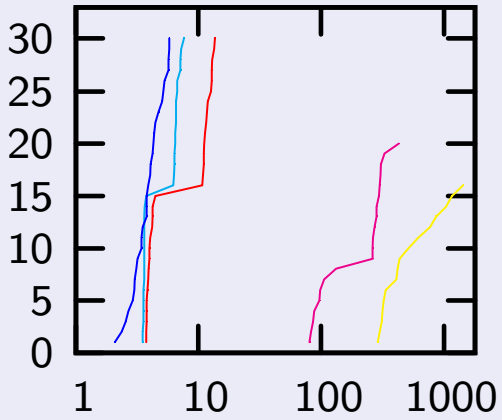
Latin Square



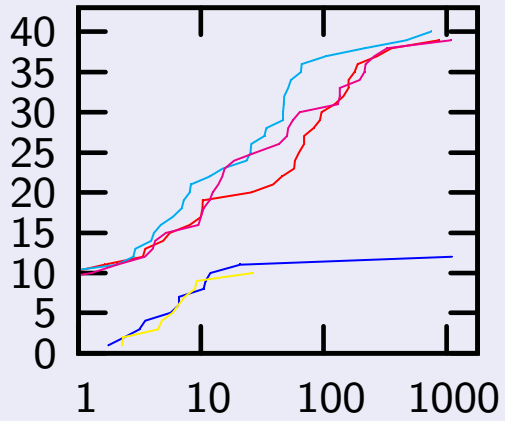
Social Golfer



Bnd Span Tree



Blocked Queens



Key

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Practical Performance Needs

Logicians: done when we have a correct axiomatization.

Customers: people want instances solved, not axiomatized.

To solve hard search problems, we must help the solver!

Axiomatization Techniques for Performance

Some basic techniques:

- Eliminating Symmetric Clauses
- Solution Symmetry Breaking
- Redundant Axioms
- Auxiliary Predicates
- Inductive Definitions as a pre-processing technique
- Bounded Quantifiers and Ordering
- Cardinality Constraints

Note: With cardinality we usually use MXC, a SAT+Cardinality solver.

Outline

Larger Example: "Phylogenetic Reconstruction"

- Given species data, construct an evolutionary tree that explains it
- Many variants – most NP-Complete
- Declarative solutions would be very useful

The Binary Camin-Sokal Problem (BCS)

INSTANCE:

- Set S of n distinct vectors from $\{0,1\}^m$;
- Natural number B.

QUESTION: Is there a directed tree $T = (V, E)$, such that:

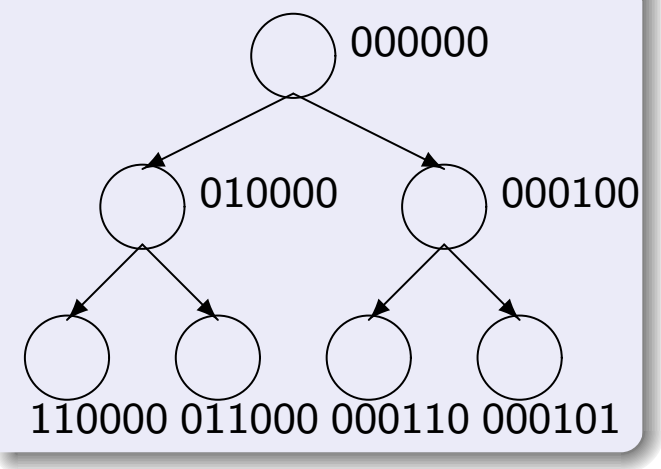
- T is rooted at 0^m;
- $S \subseteq V \subseteq \{0,1\}^m$;
- Every leaf of T is in S;
- For each directed edge $(v_1, v_2) \in E$, v_1 and v_2 differ in exactly one character, which is 0 at v_1 and 1 at v_2;
- $|V| \leq B$.

The Binary Camin-Sokal Problem (BCS)

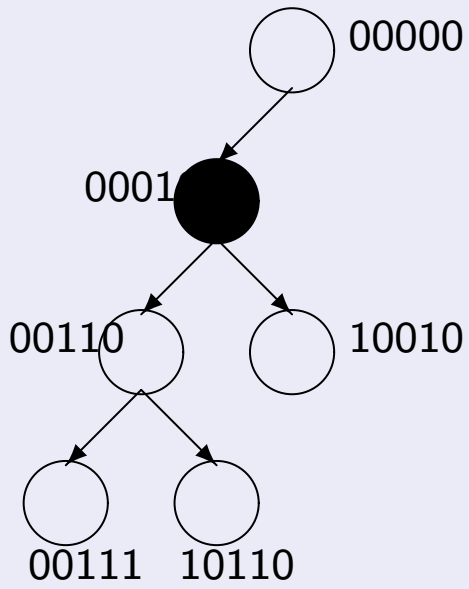
Perfect Phylogeny, each character mutates *exactly once*

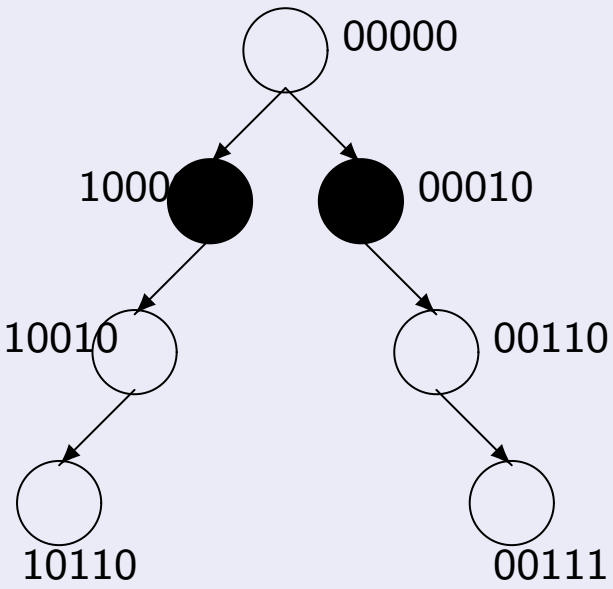
(# Nodes = # Characters + 1)

Perfect Phylogeny



Optimal and Sub-Optimal Trees





Conflict: 4 species covering $\{00, 01, 10, 11\}$ for some pair of characters

Requires one species appear in two distinct sub-trees

Basic MX Axiomatization of BCS

```
Given:
    type   Char State Vertex;
    A(Vertex, Char, State)   // Species Data
    NSpecies: Vertex
    NEdges: Vertex

Find:
    Edge(Vertex, Vertex)   // The Tree
    Vector(Vertex, Char)    // Vectors labeling vertices

Satisfying:
```

Basic MX Axiomatization of BCS

Continued

Each edge has exactly one mutation, which is $0 \longrightarrow 1$

$\forall$ u v : Edge(u,v) $\supset$ ($\exists$c : ($\neg$Vector(u,c) $\wedge$ Vector(v,c)))

$\forall$ u v : UB(1; c; (Edge(u,v) $\wedge$ $\neg$Vector(u,c) $\wedge$ Vector(v,c)))

$\forall$ u v : UB(0; c; (Edge(u,v) $\wedge$ Vector(u,c) $\wedge$ $\neg$Vector(v,c)))

Edge represents a tree rooted at $\vec{0}$

CARD(NEdges; v, u; Edge(v,u))

$\forall$ v $>$ MIN : CARD(1; u; Edge(u, v))

First *n* vertices labeled with species data

$\forall$ s $\leq$ NSpecies c : (A(s,c,MAX) $\Leftrightarrow$ Vector(s, c))

Measuring Progress

Instances:

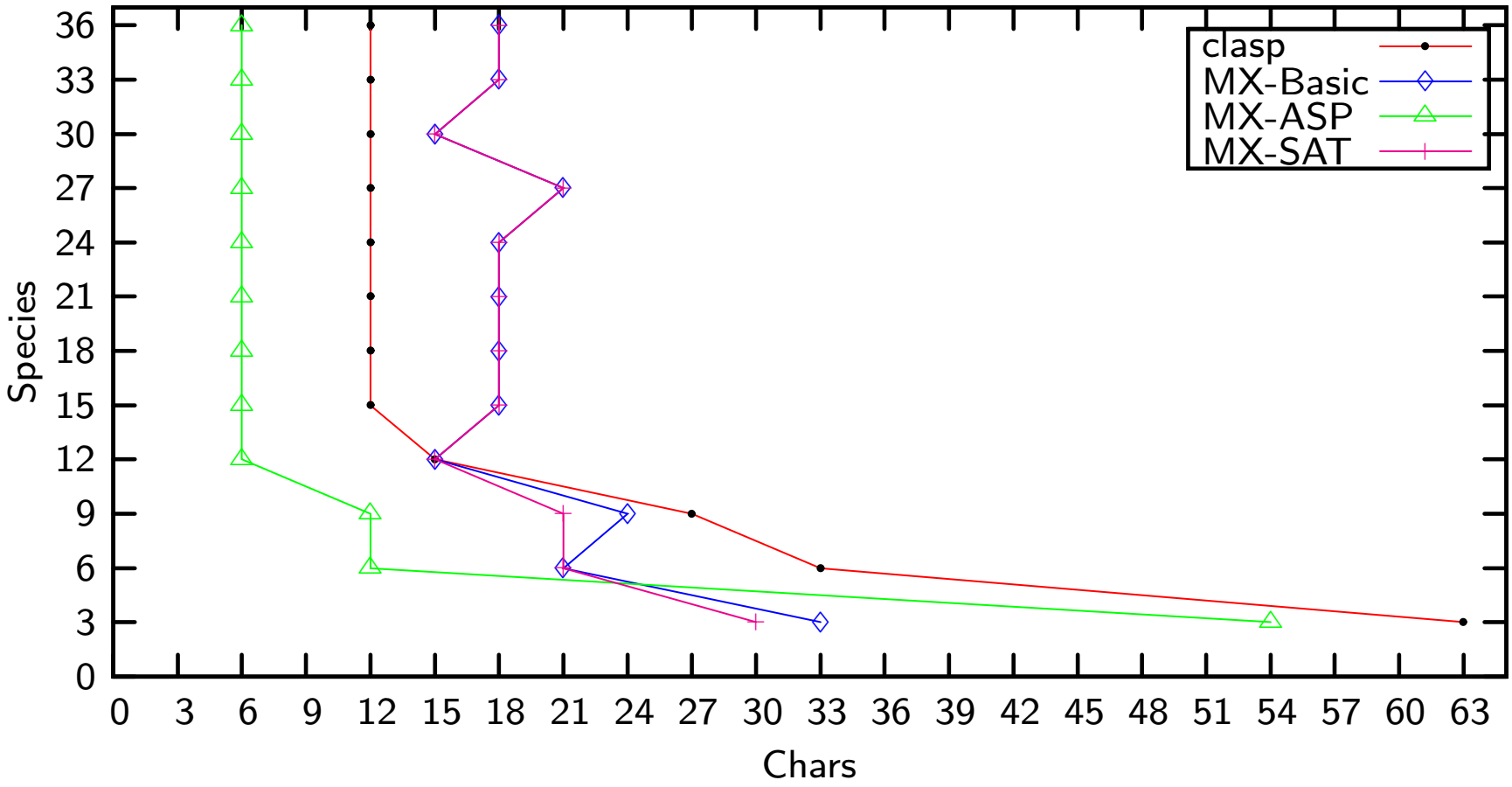
- Real Data Set: 37 Species, 65 Characters, 2 States
- Graduated instances:
  - subsets with first k species; first l characters (for k, l multiples of 3).
  - Let $\vec{0}$ be the first species; put other in reverse lexicographic order. (Species 2 has many 1's.)

Measuring Performance:

- Solve to Optimality (solve a sequence of instances)
- Plot maximum size solved to optimality in 2 hours

MXG *vs* Previous ASP Solution

Answer Set Programming: Specification with Logic Programming Rules
clasp: Very fast ASP solver



Improving Performance: Redundant Axioms (Depth)

FACT: In a BCS tree, a vector with k 1's must be at depth k
Make the property explicit with redundant axioms:

Each vertex has a unique depth

$\forall$ u : CARD(1; d; VtxDepth(u, d))

Depth difference between a child and a parent is 1

$\forall$ u v d1 d2 : ((Edge(u,v) $\wedge$ VtxDepth(u, d1) $\wedge$ VtxDepth(v,d2))
$\supset$ SUCC(d1, d2))

A species must be at it's correct depth

$\forall$ u$\leq$NSpecies d: (VtxDepth(u,d) $\Leftrightarrow$ SpcDepth(u,MAX,d))

Further Axioms (DepthPlus)

Only the root is at depth 0

$\forall$ u>MIN : $\neg$ VtxDepth(u,MIN)

"extra" vertices are ordered by depth (Symmetry Breaking Axiom)

$\forall$ u>NSpecies v>u d1 d2 : ((VtxDepth(u,d1) $\wedge$ VtxDepth(v,d2))
$\supset$ d2 $\geq$ d1)

"extra" vertices are not leaves (not quite redundant – but very helpful)

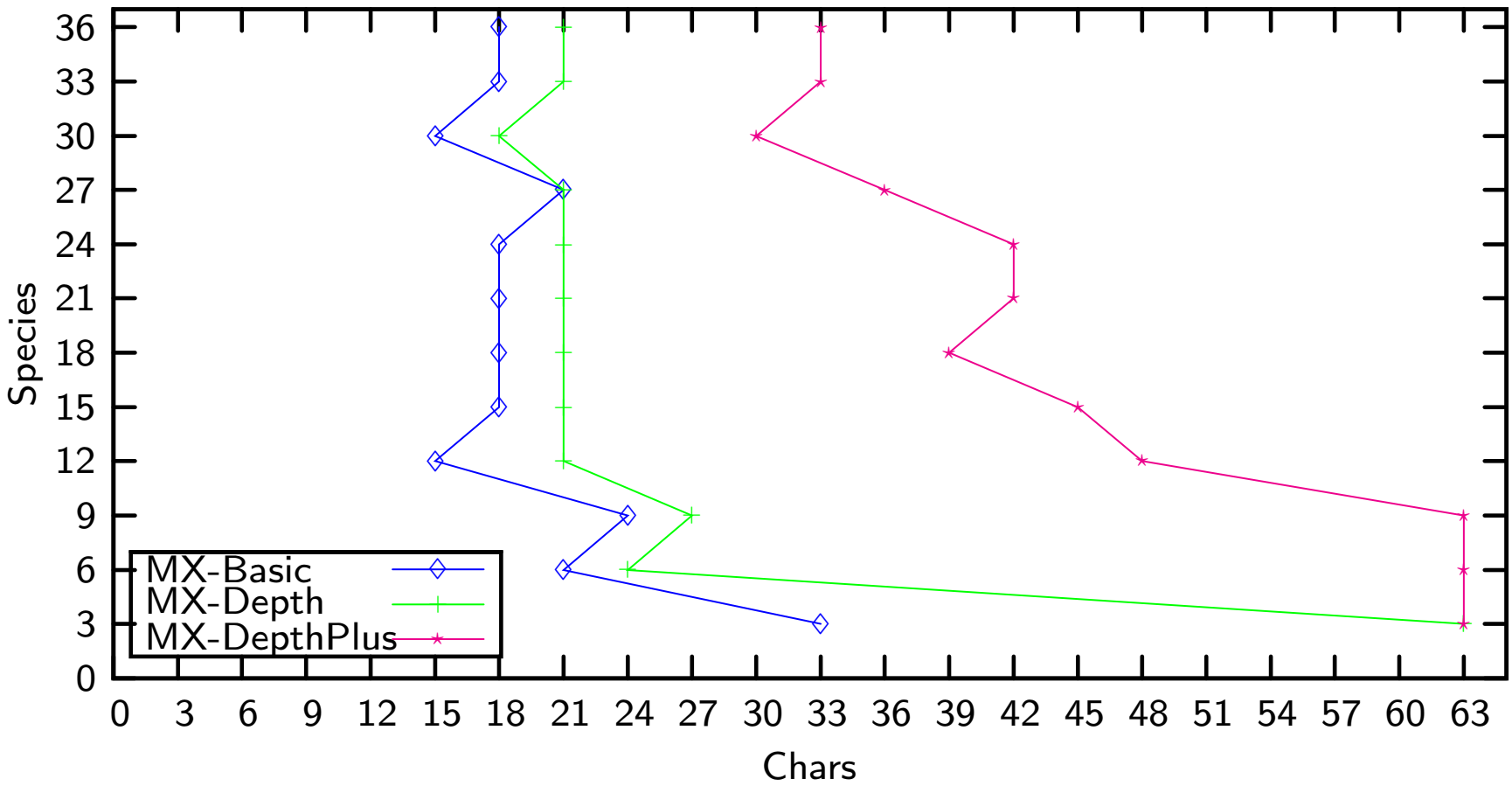
$\forall$ u>NSpecies : $\exists$ v : Edge(u,v)

Redundant Axioms - Pre-Computing Depth

MXG Computes this Definition while grounding
It determines the depth of each species vector

$$
\begin{aligned}
\{\ & \mathrm{SpcDepth(u,c,d)} \leftarrow \mathrm{c{=}MIN} \wedge \mathrm{d{=}MIN} \wedge \mathrm{s} = \mathrm{MIN} \wedge \mathrm{A(u,c,s)} \\
& \mathrm{SpcDepth(u,c,d)} \leftarrow \mathrm{c{=}MIN} \wedge \mathrm{SUCC(MIN,\ d)} \\
& \qquad\qquad \wedge\ \mathrm{s} = \mathrm{MAX} \wedge \mathrm{A(u,c,s)} \\
& \mathrm{SpcDepth(u,c,d)} \leftarrow \mathrm{SpcDepth(u,c1,\ d)} \wedge \mathrm{SUCC(c1,\ c)} \\
& \qquad\qquad \wedge\ \mathrm{A(u,c,s)} \wedge \mathrm{s{=}MIN} \\
& \mathrm{SpcDepth(u,c,d)} \leftarrow \mathrm{SpcDepth(u,c1,\ d1)} \wedge \mathrm{SUCC(c1,c)} \\
& \qquad\qquad \wedge\ \mathrm{SUCC(d1,\ d)} \wedge \mathrm{A(u,c,s)} \wedge \mathrm{s{=}MAX} \\
\}
\end{aligned}
$$

Performance of Refined Axiomatizations

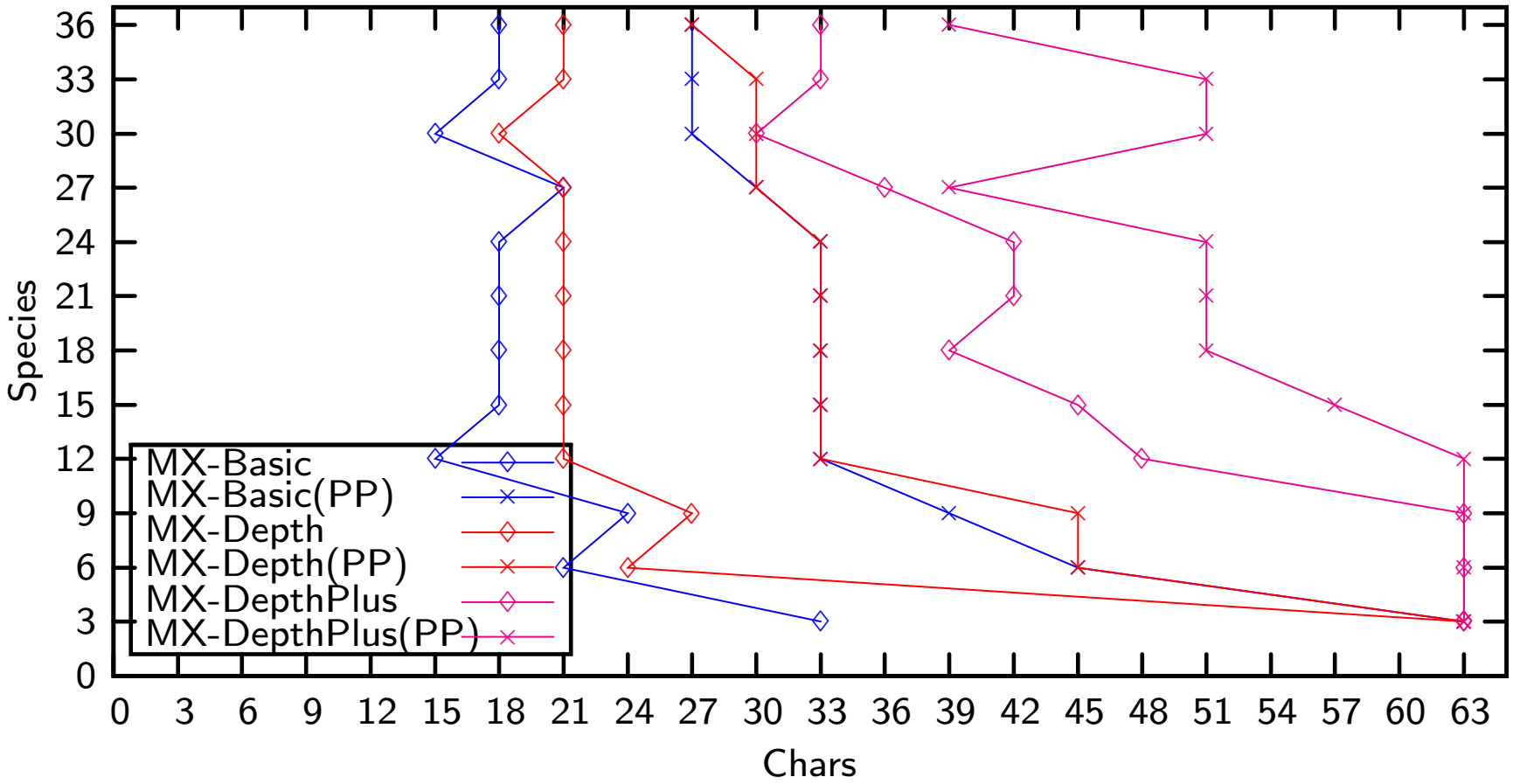


Instance Pre-Processing

We recursively applied the following rules:

- Delete any all-zero column.
- Delete any column having exactly one 1.
- Delete any column having exactly one 0.
- Delete any duplicate species.
- Delete s_2 for any pair s_1, s_2 of species such that:
  - $s_1 \subset s_2$, i.e., every character that is 1 for s_1 is also 1 for s_2;
  - $|s2 - s1| = k$, i.e., s_2 has k more 1's than s_1;
  - $\forall s_3 \notin \{s_1, s_2\}, |s_2 \backslash s_3| \geq k$.

Performance of Refined Axiomatizations



These changes reflect many orders of magnitude difference in run times.

Outline

Conclusions

Our experience to date indicates:

- FO(ID)-MX and our grounding/solving method are feasible approach to NP Search.
- MXG is competitive with high-quality ASP solvers.
- We can refine performance of MXG by:
  - usual techniques of declarative programming (at specification level),
  - specific features of MXG.
- Using a modelling language front end can be effective:
  - quickly produce reasonable solutions
  - efficiently try multiple representations
  - effectively refine to obtain good performance
  - de-bugging is more efficient than with standard methodology
- Good performance can be obtained:
  - with logic-based tools
  - without ad-hoc restrictions on language
- Poly-time instance pre-processing can be done declaratively
- We also found MXG a useful SAT solver debugging aid!

Future Work

- Language Extensions (i.e., arithmetic, strings, matrices)
- Improved Grounding (i.e., generalize query optimization)
- Specification Pre-processing (i.e., symmetry detection)
- Other Ground Solvers (i.e., SMT, PB, ILP)
- Extend to Optimization Problems
- Handle unrestricted inductive definitions
- Further Evaluation:
  - wider range of problems
  - other competing technologies (CLP, CSP, ILP, ...)

Credits

MX Project Principals:

- Eugenia Ternovska,
- David G. Mitchell

MXG Implementation and Demonstration:

- Raheleh Mohebali,
- Faraz Hach

MXC SAT Solver:

- David Bregman

Others:

- Yongmei Liu, Arvind Gupta, Murray Patterson, Jonathan Kavanagh, Jano Manuch, Sharon Xiao, Nhan Nguyen, Brendan Guild, Nikolay Pelov, ...

Links and References

- MX Project Web Site: www.cs.sfu.ca/research/groups/mxp/
  (painfully out of date)
- Abstraction and Expressiveness in Essence

  M., Ternovska — Constraints (to appear)
- Declarative Programming for Search Problems with Built-in Arithmetic

  Ternovska, M.
- Faster Phylogenetic Inference with MXG

  M., Hach, Mohebali — LPAR'07
- Constructing Camin-Sokal Phylogenies via Answer Set Programming

  Kavanagh, M., Ternovska, Manuch, Zhao, Gupta — LPAR'06
- A Framework for Modelling and Solving Search Problems

  M., Ternovska, Hach, Mohebali — SFU CS TR 2006-24
- A Framework for Representing Search Problems

  M., Ternovska — AAAI'05