Algorithmic Algorithm Synthesis:

Case Study Gröbner Bases

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Dedicated to Bob F. Caviness

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Outline:

The Theorema Project

An "Algorithm" for Algorithm Synthesis

Synthesis of a Gröbner Bases Algorithm

Conclusion

The Theorema Project

An Algorithm for Algorithm Synthesis

Algorithmic Synthesis of a Gröbner Bases Algorithm

Conclusion

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■ Current Mathematical Knowledge

- o algorithm libraries, e.g. Mathematica, Maple, etc.
- o decision algorithms and proof generators for certain logical theories
- o proof checkers and proof generators for predicate logic
- o
- o mathematical "knowledge" in paper form, LaTeX files etc.

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■ What "We" Want

Integrated Systems

Integrated systems that support (partially automate) the entire "mathematical theory exploration" process:

Invention and Verification

Starting from some given mathematical concepts and mathematical knowledge on these concepts within a uniform logical language (predicate logic),

- o invent definitions (axioms) of new concepts
- o invent and prove / disprove propositions on these concepts
- o invent problems
- o invent and verify algorithms for problems
- store the new knowledge (definitions, propositions, problems, algorithms) in structured knowledge libraries so that they can be used easily in the next rounds of mathematical theory exploration.

□ For example:

start from: +, -, *, ..< on reals (axioms, propositions, problems, algorithms)

new concepts: definitions of "sequence" and operations +, -, ... on sequences

explore: propositions, problems, algorithms on sequences

new concepts: "limit", "continuity"

explore: propositions, problems, algorithms on sequences

A benchmark example:

Computer-supported development of the theory of Groebner bases and related theories.

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■ The *Theorema* Project

The *Theorema* project [BB et al. 1996 ...] aims at being a frame for supporting mathematical theory exploration in the above sense.

The *Theorema* language is a version of predicate logic.

A sublanguage of the *Theorema* language is a programming language.

The Theorema system is implemented in Mathematica. (This may change in the future.)

The *Theorema* group: B. B. (leader), T. Jebelean, T. Kutsia, F. Piroi, M. Rosenkranz, W. Windsteiger, and PhD students.

■ Mathematical Knowledge Management: A Recent International Endeavor

The *Theorema* group is (an initiator and member) of the international MKM (Mathematical Knowledge Management) Network (NuPrl, Izabelle, MIZAR, ...)

Numerical Mathematics

Computer Algebra

Automated Theorem Proving

Mathematical Knowledge Management ("Symbolic Computation" in its widest sense)

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■ The Algorithm Invention ("Synthesis") Problem

Given a problem specification P (in predicate logic), find an algorithm A such that

$$\forall_{x} P[x, A[x]].$$

Examples of specifications P:

```
P[x, y] ⇔ is-greater[x, y]

P[x, y] ⇔ is-sorted-version[x, y]

P[x, y] ⇔ has-derivative[x, y]

P[x, y] ⇔ are-factors-of[x, y]

P[x, y] ⇔ is-Gröbner-basis[x, y]
```

A general algorithm S for "all" P cannot exist (cf. B. Caviness 1970, ...) but ...

There is a rich literature on algorithm synthesis methods.

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■ The "Lazy Thinking" Method (BB 2001): A Very Rough Sketch

Given: a problem specification P.

For finding an algorithm A that satisfies $\forall P[x, A[x]]$,

- we generate (automatically) a couple of (hopefully) simpler problems Q, R, ...,
- we synthesize algorithms B, C, ... for Q, R, ...
- from B, C, ... we compose (automatically) an algorithm A.

When can we terminate?

When we arrive at problems, for which algorithms are already known.

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■ The "Lazy Thinking" Method: More Details

Given a problem specification P

- o consider various "algorithm schemes" for A
- o and try to prove (automatically) $\forall P[x, A[x]]$.
- This proof will normally fail because nothing is known on the unspecified sub-algorithms in the algorithm scheme.
- From the temporary assumptions and goals in the failing proof situation (automatically) generate such specifications for the unspecified sub-algorithms that would make the proof possible.

Now, apply the method recursively to the auxiliary functions.

- □ This is "lazy"
 - o we use the condensed algorithmic experience of others (in the schemes)
 - o we start (routine) proving before we have an algorithm
 - o we just wait until we fail in order to get an idea from the failure.

■ Example: Synthesis of Merge-Sort [BB et al. 2003]

□ Problem

Synthesize "sorted" such that

```
\forall is-sorted-version[x, sorted[x]].
```

("Correctness Theorem")

Knowledge on Problem

```
\forall_{\mathtt{x},\mathtt{y}} \; \Big( \mathtt{is-sorted-version}[\mathtt{x},\,\mathtt{y}] \; \Leftrightarrow \; \begin{matrix} \mathtt{is-sorted}[\mathtt{y}] \\ \mathtt{is-permuted-version}[\mathtt{x},\,\mathtt{y}] \end{matrix}\Big)
```

$$\forall_{\mathtt{x},\mathtt{y}} \; \Big(\mathtt{is}\mathtt{-sorted} \Leftrightarrow \underbrace{\mathtt{is}\mathtt{-sorted}[\mathtt{y}]}_{\mathtt{is}\mathtt{-permuted}\mathtt{-version}[\mathtt{x},\;\mathtt{y}]} \Big)$$

is-sorted[()]

∀ is-sorted[⟨x⟩]

$$\forall_{\mathtt{x},\mathtt{y},\bar{\mathtt{z}}} \; \Big(\mathtt{is}\text{-sorted}[\langle \mathtt{x},\,\mathtt{y},\,\bar{\mathtt{z}}\rangle] \Leftrightarrow \frac{\mathtt{x} \geq \mathtt{y}}{\mathtt{is}\text{-sorted}[\langle \mathtt{y},\,\bar{\mathtt{z}}\rangle]} \Big)$$

etc.

An Algorithm Scheme

```
\[
\frac{\formalfont{\text{special}[x]}}{\text{special}[x]} & \text{is-trivial-tuple[x]} \\
\[
\begin{cases} \text{merge[sorted[left-split[x]], sorted[right-split[x]]]} & \text{cotherwise} \\
\end{cases}
\]
\[
\text{definition of the point of the
```

("divide and conquer")

We Now Start Proving the Correctness Theorem and Analyze the Failing Proof

The Result of Applying Lazy Thinking

Lazy Thinking, automatically (in approx. 2 minutes on a laptop using the *Theorema* system), finds the following specifications for the sub-algorithms that provenly guarantee the correctness of the above algorithm (scheme):

```
∀ (is-trivial-tuple[x] ⇒ special[x] = x)

∀ (is-sorted[y] ⇒ is-sorted[merged[y, z]])
∀ (is-sorted[z] ⇒ merged[y, z] ≈ (y ≈ z)

∀ (left-split[x] ≈ right-split[x] ≈ x)
```

What Do We Have Now?

- Case A: We find algorithms special, merged, left-split, right-split in our knowledge base for which the properties specified above are already contained in the knowledge base or can be derived from the knowledge base.
 - In this case, we are done, i.e. we have synthesized a sorting algorithm.
- Case B: We do not find algorithms special, merged, left-split, right-split in our knowledge base for which the properties specified can be proved.
 In this case, we apply Lazy Thinking again in order to synthesize appropriate special, merged,

In this case, we apply Lazy Thinking again in order to synthesize appropriate special, merged, left-split, right-split

until we arrive at sub-sub-...-algorithms in our knowledge base (e.g. the basic operations of tuple theory like append, prepend etc.)

Case B can be avoided, if we proceed systematically bottom-up ("complete theory exploration" in layers).

■ How Can we Teach (= Automate) the Method

- o Compile a library of "algorithm design experience" (= algorithm schemes).
- o Teach (automate) proving.
- Teach (automate) generation of useful specifications of sub-algorithms from failing correctness proofs:

A simple (but amazingly powerful) rule:

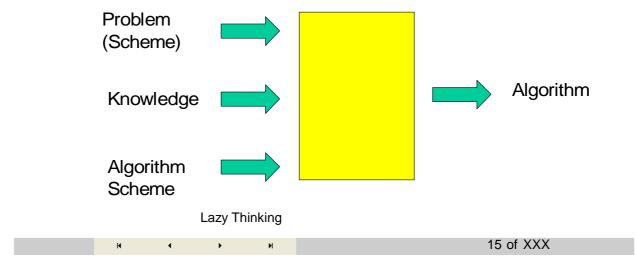
Collect temporary assumptions T[x0, ...A[], ...] and temporary goals G[x0, ...m[A[]]] and produces specification

$$\forall_{X,\ldots,Y,\ldots} (T[X,\ldots Y,\ldots] \Rightarrow G[Y,\ldots m[Y]]).$$

Details: see papers [BB 2003] and example.

Research topic: other rules.

■ Parameters for Lazy Thinking



■ Example: Synthesis of Insertion-Sort

Problem

Synthesize A such that

```
\forall is-sorted-version[x, A[x]].
```

Algorithm Scheme: "simple recursion"

```
A[\langle \rangle] = C
\forall A[\langle x \rangle] = S[\langle x \rangle]
\forall (A[\langle x, \bar{y} \rangle] = i[x, A[\langle \bar{y} \rangle]])
x, \bar{y}
```

Resulting Specification for Subalgorithms

Lazy Thinking, automatically (in approx. 2 minutes on a laptop using the *Theorema* system), finds the following specifications for the auxiliary functions

```
\begin{array}{l} \mathbf{C} = \langle \rangle \\ \forall \quad (\mathbf{S}[\langle \mathbf{x} \rangle] = \langle \mathbf{x} \rangle) \\ \forall \quad \forall \quad (\mathbf{is} - \mathbf{sorted}[\langle \bar{\mathbf{y}} \rangle] \Rightarrow \mathbf{is} - \mathbf{sorted}[\mathbf{i}[\mathbf{x}, \langle \bar{\mathbf{y}} \rangle]] \\ \forall \quad \forall \quad (\mathbf{x}, \bar{\mathbf{y}}) \Rightarrow \mathbf{i}[\langle \mathbf{x}, \bar{\mathbf{y}} \rangle] \approx (\mathbf{x} - \langle \bar{\mathbf{y}} \rangle) \end{array}
```

Details of an Automated Synthesis

See the notebooks automatically produced by *Theorema* for the insertion-sort example.

■ How far can we go with this method?

Can we automatically synthesize algorithms for non-trivial problems?

Example of a non-trivial problem: construction of Gröbner bases.

What is "non-trivial"?

Main algorithmic idea of Gröbner bases theory: The "S-polynomials" ("critical pairs") together with the S-polynomial theorem.

Hence, question: Can Lazy Thinking automatically invent the notion of S-polynomial and automatically deliver the S-polynomial theorem.

- √ What we Have, What we Want
- ✓ An Algorithm for Algorithm Synthesis

Algorithmic Synthesis of a Gröbner Bases Algorithm

Conclusion

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■ The Problem of Constructing Gröbner Bases

Find algorithm Gb such that

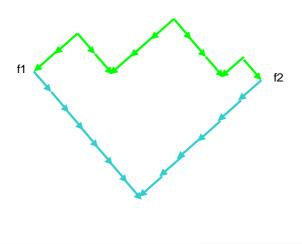
Definitions [BB 1965, 1970]:

```
is-Gröbner-basis[G] \Leftrightarrow is-confluent[\rightarrow_G].
```

■ Confluence of Division →_G

$$(\text{h1} \rightarrow_{\text{g}} \text{h2}) \Leftrightarrow \exists \atop \text{geG}} \left(\left\{ \begin{matrix} \text{lp[g]} \mid \text{lp[h1]} \\ \text{h2} = \text{h1} - (\text{lm[h1]} / \text{lm[g]}) \text{ g} \end{matrix} \right),\right.$$

$$\texttt{is-confluent}[\,\rightarrow\,]\;:\;\Leftrightarrow\;\forall_{\texttt{fl},\texttt{f2}}\;(\texttt{f1}\leftrightarrow^*\texttt{f2}\Rightarrow\texttt{f1}\downarrow^*\texttt{f2})$$



■ Knowledge on the Concepts Involved

$$h1 \rightarrow_G h2 \Rightarrow p \cdot h1 \rightarrow_G p \cdot h2$$

etc.

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■ Algorithm Scheme "Critical Pair / Completion"

$$\begin{split} &\mathbf{A}[\mathbf{F}] = \mathbf{A}[\mathbf{F}, \, \mathsf{pairs}[\mathbf{F}]] \\ &\mathbf{A}[\mathbf{F}, \, \langle \, \rangle] = \mathbf{F} \\ &\mathbf{A}[\mathbf{F}, \, \langle \, \langle \mathsf{g1}, \, \mathsf{g2} \rangle, \, \bar{p} \rangle] = \\ &\text{where} \big[\mathbf{f} = \mathbf{lc}[\mathsf{g1}, \, \mathsf{g2}], \, \mathbf{h1} = \mathsf{trd}[\mathsf{rd}[\mathsf{f}, \, \mathsf{g1}], \, \mathbf{F}], \, \mathbf{h2} = \mathsf{trd}[\mathsf{rd}[\mathsf{f}, \, \mathsf{g2}], \, \mathbf{F}], \\ & \left\{ \begin{aligned} &\mathbf{A}[\mathbf{F}, \, \langle \bar{p} \rangle] & \leftarrow & \mathbf{h1} = \mathbf{h2} \\ &\mathbf{A}[\mathbf{F} \circ \mathsf{df}[\mathsf{h1}, \, \mathsf{h2}], \, \langle \bar{p} \rangle \times \left\langle \langle \mathbf{F}_k, \, \mathsf{df}[\mathsf{h1}, \, \mathsf{h2}] \rangle \, \big|_{k=1,\dots,|\mathbf{F}|} \right\rangle \right] & \leftarrow & \text{otherwise} \end{aligned} \right] \end{split}$$

This scheme can be tried in any domain, in which we have a reduction operation rd that depends on sets F of objects and a Noetherian relation > which interacts with rd in the following natural way:

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■ The Essential Problem

The problem of synthesizing a Gröbner bases algorithm can now be also stated by asking whether starting with the proof of

```
is-finite[A[F]]
is-Gröbner-basis[A[F]]
ideal[F] = ideal[A[F]].
```

we can automatically produce the idea that

```
lc[g1, g2] = lcm[lp[g1], lp[g2]]
```

and

$$df[h1, h2] = h1 - h2$$

and prove that the idea is correct.

■ Now Start the (Automated) Correctness Proof

With current theorem proving technology, in the *Theorema* system, the proof attempt could be done automatically. (Not yet fully implemented.)



■ Details

Upon Termination

It should be clear that, if the algorithm terminates, the final result is a finite set (of polynomials) G that has the property

$$\forall _{g1,g2 \in G} \text{ (where [f = lc[g1, g2], h1 = trd[rd[f, g1], F], }$$

$$h2 = trd[rd[f, g2], F], \bigvee \left\{ \begin{matrix} h1 = h2 \\ df[h1, h2] \in G \end{matrix} \right] \right).$$

We Have to Prove

We now try to prove that, if G has this property, then

```
is-finite[G],
ideal[F] = ideal[G],
is-Gröbner-basis[G],
i.e. is-Church-Rosser[→<sub>G</sub>].
```

Here, we only deal with the third, most important, property.

Using Available Knowledge

Using Newman's lemma and some elementary properties it can be shown that it is sufficient to prove

$$\text{is-Church-Rosser[} \rightarrow_{\text{G}} \text{]} \Leftrightarrow \bigvee_{\text{p}} \bigvee_{\text{fl,f2}} \left(\left(\left\{ \begin{matrix} p \rightarrow \text{fl} \\ p \rightarrow \text{f2} \end{matrix} \right. \right) \Rightarrow \text{f1} \downarrow^{*} \text{f2} \right).$$

Assumption

Let now the power product p and the polynomials f1, f2 be arbitary but fixed and assume

$$\begin{cases} p \rightarrow_G f1 \\ p \rightarrow_G f2. \end{cases}$$

We have to find a polyonomial g such that

f1
$$\rightarrow_G^* g$$
,
f2 $\rightarrow_G^* g$.

From the Assumption

From the assumption we know that there exist polynomials g1 and g2 in G such that

```
lp[g1] | p,
f1 = rd[p, g1],
lp[g2] | p,
f2 = rd[p, g2].
```

From the final situation in the algorithm scheme we know that for these g1 and g2

```
\bigvee \left\{ \begin{array}{l} h1 = h2 \\ df[h1, h2] \in G, \end{array} \right.
```

where

```
h1 := trd[f1', G], f1' := rd[lc[g1, g2], g1],
h2 := trd[f2', G], f2' := rd[lc[g1, g2], g2].
```

Case h1=h2: In this case

```
lc[g1, g2] \rightarrow_{g1} rd[lc[g1, g2], g1] \rightarrow_{G}^{*} trd[rd[lc[g1, g2], g1], G] = trd[rd[lc[g1, g2], g2], G] \leftarrow_{G}^{*} rd[lc[g1, g2], g2] \leftarrow_{g2} lc[g1, g2].
```

(Note that here we used the requirements rd[lc[g1,g2],g1] < lc[g1,g2] and rd[lc[g1,g2],g2] < lc[g1,g2].)

Hence, by elementary properties of polynomial reduction,

```
\begin{array}{c} \forall & (\ a \ q \ l \ c \ [g1, \ g2] \ \rightarrow_{g1} \\ & \ a \ q \ r \ d \ [l \ c \ [g1, \ g2] \ , \ g1] \ \rightarrow_{G}^* \ a \ q \ t \ r \ d \ [l \ c \ [g1, \ g2] \ , \ g2] \ \leftarrow_{g2} \\ & \ a \ q \ l \ c \ [g1, \ g2] \ ) \ . \end{array}
```

Now we are stuck in the proof.

Use Specification Generation Algorithm

However, using the above specification generation rule, we see that we could proceed successfully with the proof if lc[g1,g2] satisfied the following requirement

$$\forall \left(\left(\left\{ \begin{array}{l} lp[g1] \mid p \\ lp[g2] \mid p \end{array} \right) \Rightarrow \left(\begin{array}{l} \exists \\ a,q \end{array} \right. (p = aqlc[g1,g2]) \right) \right), \quad (lc \, requirement)$$

With such an lc, we then would have

```
p \rightarrow_{g1} rd[p, g1] = aqrd[lc[g1, g2], g1] \rightarrow_{g}^{*} aqtrd[rd[lc[g1, g2], g1], G] = aqtrd[rd[lc[g1, g2], g2], G] \leftarrow_{g}^{*} aqrd[lc[g1, g2], g2] = rd[p, g2] \leftarrow_{g2} p
```

and, hence,

$$f1 \rightarrow_G^* aq trd[rd[lc[g1, g2], g1], G],$$

$$f2 \rightarrow_G^* aq trd[rd[lc[g1, g2], g1], G],$$

i.e. we would have found a suitable g.

Summarizing the Specifications of the Unknown Subalgorithm Ic

(Ic requirement), which also could be written in the form:

$$\forall \atop \texttt{p,g1,g2} \left(\left(\left\{ \begin{matrix} \texttt{lp[g1]} \mid \texttt{p} \\ \texttt{lp[g2]} \mid \texttt{p} \end{matrix} \right. \right) \Rightarrow \left(\texttt{lc[g1,g2]} \mid \texttt{p} \right) \right) \,,$$

and the requirements:

which, in the case of the domain of polynomials, are equivalent to

A Suitable Ic

is a suitable function that satisfies the above requirements.

Heureka! The crucial function lc (the "critical pair" function) in the critical pair / completion algorithm scheme has been "automatically" synthesized!

□ Case h1≠h2 and, hence, df[h1,h2]∈G:

In this part of the proof we are basically stuck right at the beginning.

We can try to reduce this case to the first case, which would generate the following requirement

$$\forall_{\text{h1,h2}} (\text{h1} \downarrow_{\{\text{df[h1,h2]}\}}^* \text{h2}) \quad (\text{df requirement}).$$

(Looking to the knowledge base of elementary properties of polynomial reduction, it is now easy to find a function df that satisfies (df requirement), namely

$$df[h1, h2] = h1 - h2,$$

because, in fact,

Heureka! The function df (the "completion" function) in the critical pair / completion algorithm scheme has been "automatically" synthesized!)

Namely,

■ Summary of the Synthesizing Proof Attempt

Failure Situation

The proof, of course, fails at the point where it would need knowledge about the unknown subalgorithms lc and df.

Beginning of the proof:

Let G be A[F]. We have to prove that

```
is-finite[G],
ideal[F] = ideal[G],
is-Gröbner-basis[G],
    i.e. is-confluent[→G].
```

Assumption

We only deal with the third, most important, property. For this, we assume

$$\begin{cases} p \to_G f1 \\ p \to_G f2. \end{cases}$$

and have to find a polynomial g such that

f1
$$\rightarrow_G$$
* g,
f2 \rightarrow_G * g.

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■ Generation of the Specification of Ic

In the failing proof situation, by the (automated) analysis algorithm sketched above, we detect that the proof could be completed if the unknown **Ic** satisfied the following property:

$$\forall \atop \mathtt{p},\mathtt{g1},\mathtt{g2}} \left(\left(\left\{ \begin{matrix} \mathtt{lp}[\mathtt{g1}] \mid \mathtt{p} \\ \mathtt{lp}[\mathtt{g2}] \mid \mathtt{p} \end{matrix} \right. \right) \Rightarrow \left(\begin{matrix} \mathtt{lc}[\mathtt{g1},\mathtt{g2}] \mid \mathtt{p} \end{matrix} \right) \right) .$$

Eureka! It is clear that this specification is (only) met by

```
lc[g1, g2] = lcm[lp[g1], lp[g2]].
```

■ Generation of the Specification of df

Similarly, it can be (automatically) detected that

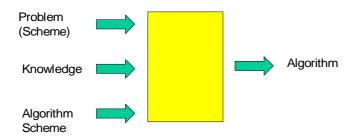
$$df[h1, h2] = h1 - h2.$$

- √ What we Have, What we Want
- ✓ An Algorithm for Algorithm Synthesis
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Conclusion

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■ Research Topics



• Libraries of algorithm schemes.

More generally, libraries of definition, theorem, problem, and algorithm schemes.

- o Case studies of problem (schemes), knowledge, algorithm schemes and how they produce algorithms.
- o Improved algorithms for generating problem specifications from failing proofs.
- o "Functor" knowledge: each algorithm is a "functor"

If s, m, I, r is a merge structure then A is a sort structure. and A results from s, m, I, r by divide and conquer

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