# The Spirit Of The Undertaking: Origins In Macsyma And Dendral

6.871-- Lecture 3

# MACSYMA: Symbolic Mathematics

- Goals of the Project
- System Description
- Lessons

# Goals of Project

*To help applied mathematicians in solving problems*

$$\int \frac{x^4}{\left(1 - x^2\right)^{\frac{5}{2}}} = \arcsin(x) - \tan(\arcsin(x)) + \frac{1}{3}\tan^3(\arcsin(x))$$

# Symbolic Mathematics: AI Approaches

- Slagle: SAINT
- Moses: SIN
- Moses and Martin: MACSYMA
- Reduce-II
- Mathematica

# SAINT: Symbolic Automatic Integrator

$$\int \frac{x^4}{\left(1 - x^2\right)^{\frac{5}{2}}} dx$$

Try *y* = *arcsin x,* yielding:

$$\int \frac{\sin^4 y}{\cos^4 y} dy$$

$$\int \frac{\sin^4 y}{\cos^4 y} dy$$

three possible ways to deal with this:

$$\int \frac{\sin^4 y}{\cos^4 y} dy$$

three possible ways to deal with this:

$$\int \tan^4 y dy \qquad \int \cot^{-4} y dy \qquad \int 32 \frac{z^4}{(1+z^2)(1-z^2)^4} dz$$

(from z = tan(y/z))

# SAINT

- Steps
  - 26 standard forms (1-step solutions, tables)
  - 8 Algorithmic transforms (eg. sum of integrals)
  - 10 Heuristic transforms, of which derivative divides is "the most successful"
    - Goals evaluated on depth of integrand
    - Ex., $xe^{x^2}$ is of depth 3

# SAINT

- Worked like the average engineer, i.e., lots of search and backtracking
- Conceived of in terms of search, worked *because* of that. The power comes from:
  - Problem decomposition
  - Methodical exploration of alternatives
  - Looking far, wide, and deep
  - Speedy tree construction, search, backtracking
- Success is just a matter of trying enough alternatives

# SAINT

Some interesting statistics:

*Saint's Average Performance*

| | Subgoals | Unused Subgoals | Level | Heuristic Level |
|---|---|---|---|---|
| 32 Author problem | 6.4 | 2.0 | 3.5 | 1.0 |
| 52 MIT Problems | 4.7 | 0.8 | 2.9 | .8 |
| 84 Problems | 5.3 | 1.25 | 3.0 | .9 |

# The Mindset Shift

SAINT will frequently [need to] explore several paths to a solution … because it lacks the powerful machinery that SIN possesses.

One of the striking features of these programs is how little knowledge they require in order to obtain a solution. Persson in his recent thesis dealing with "sequence prediction" seems to feel that placing a great deal of context dependent information in a program would be "cheating." This emphasis seems to be useful when one desires to study certain *problem solving mechanisms* in as pure a manner as possible.

We, on the other hand, intended no such study of specific problem solving mechanisms, but mainly desired a powerful integration program <u>which behaved closely to our conception of expert human integrators</u>.

SIN, we hope, signals a return to an examination of complex problem domains.

-- Moses, 1963.
[emphasis added]

Note: almost always needed one (otherwise avg would be lower)
almost always needed exactly one (otherwise avg higher)
Can't prove that search was irrelevant, since we don't know whether earlier use of heuristics would have helped, but we should certainly be suspicious.
Also don't know whether it was the same one heuristic each time. (Even if it was a different one, it's still interesting that every problem needs one and only one heuristic.
Great example of seeing what you want to see, being mechanism driven,

# Sin

- Steps
  1. Derivative divides
  2. 11 specific methods
     - Substantial effort in deciding which to apply
     - Largely organized around recognizing the form of the problem
  3. General purpose methods (e.g., search)
- Note the sequence.
- "We feel that too few AI programs employ the fact that in many problem domains there exist methods which solve a large number of problems quickly."

# Macsyma Lessons

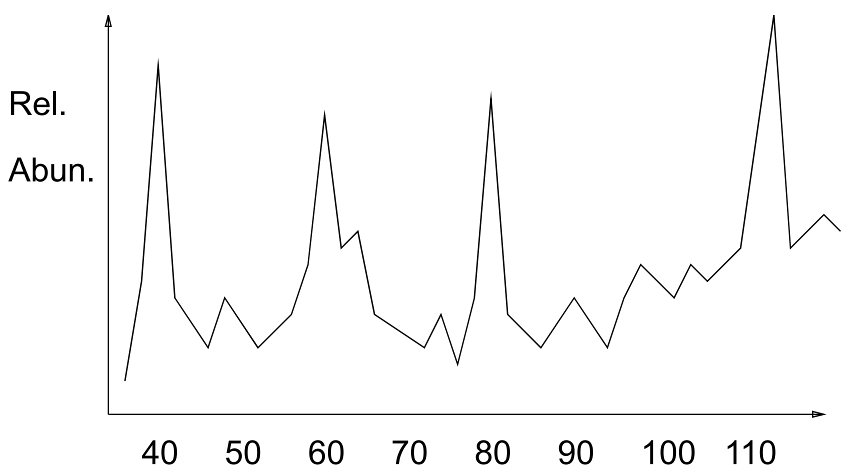
- Character of the problem changes as knowledge evolves
  - SAINT
    - Worked as people *appeared* to: extensive search and backtracking
  - SIN
    - Almost always correct on the first guess: found the sources of power in the domain
  - RISCH: Algorithmic Integration
    - Guaranteed to succeed if the expression is integrable
      - Uses very special representation
      - Computationally complex and expensive
      - Process not understandable to users but provably correct.

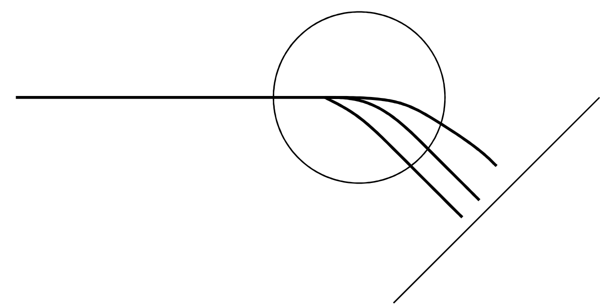
# Macsyma Lessons

- Keep the system modular and loosely coupled
  - It is sometimes cheaper to translate one representation to another in order to solve the problem more efficiently
  - Use of a common language for communication makes this approach tractable (eg, dense and sparse polynomials)
- Do not duplicate knowledge
  - leads to unmanageable system

# Dendral: Structure Elucidation

- Given:
  - Empirical Formula: $C_9H_{18}O$ (total MW = 142)
  - Known Structure Constraints
  - Mass Spectrum



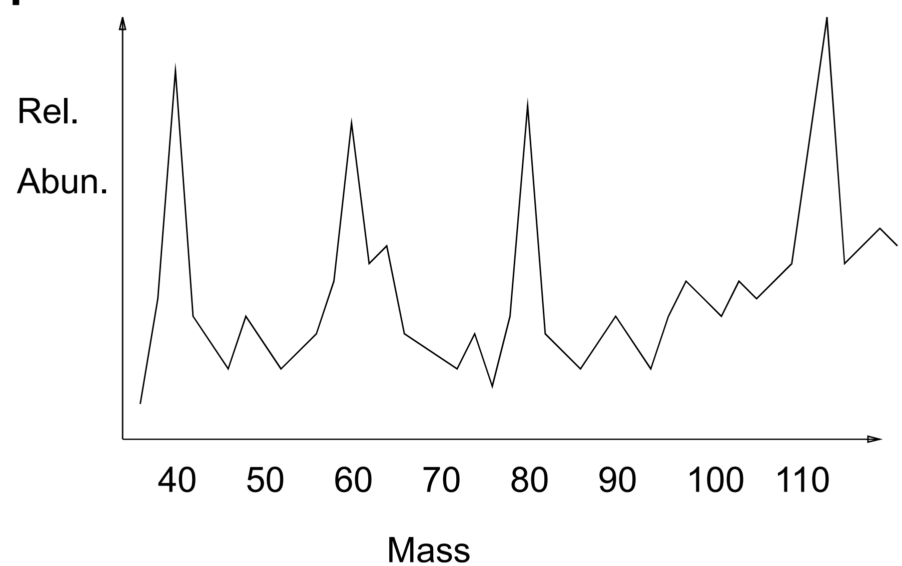



# Result

```
         O
        | |
C – C – C – C – C – C – C – C – C
```

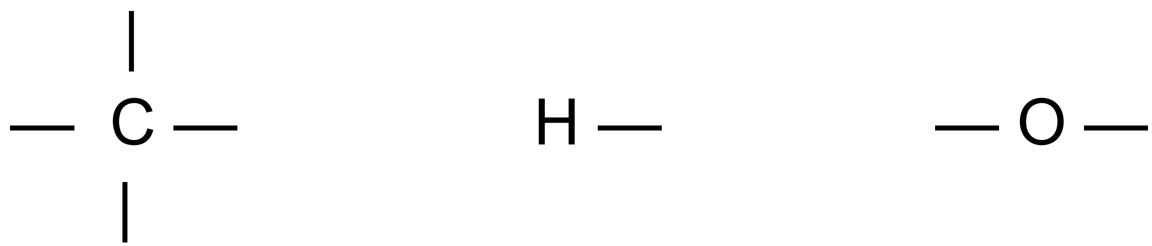
# How to Proceed?

- Given:
  - Empirical Formula: $C_9H_{18}O$ (total MW = 142)
  - Known Structure Constraints
  - Mass Spectrum

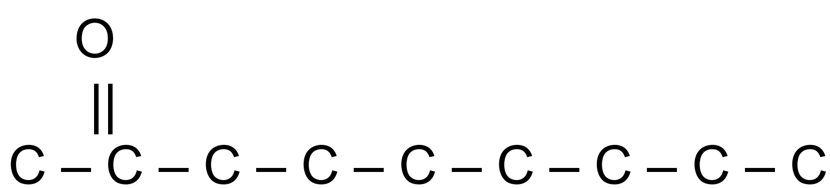


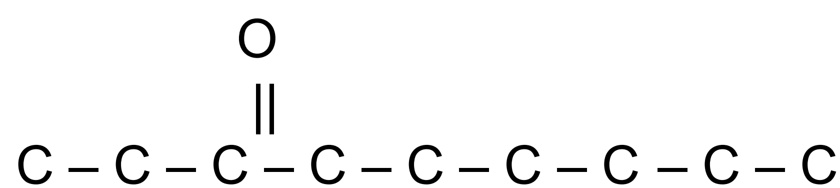

- Catalog?

# Generate and Test

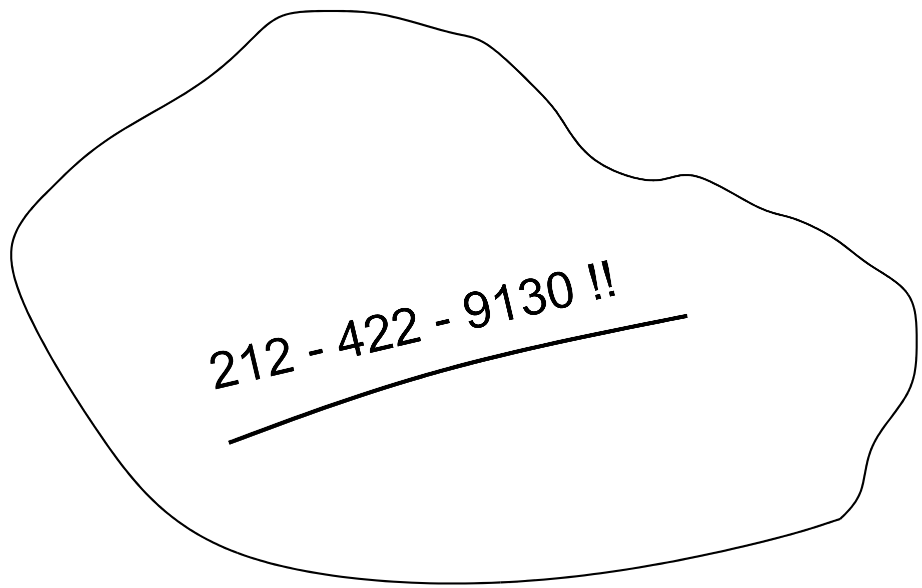


For $C_9 H_{18} O$ two possible structures are





# Difficulties in Generate & Test



# How Can the Program Plan Its Attack?

What should the program *know?*

Rules: spectrum features $\Rightarrow$ molecule class

IF There are peaks at M1 and M2 such that
M1 + M2 = MW + 28 and
M1 is high and M2 is high
THEN The structure is one of the ketones

IF There is a high peak at 44 and
there is a high peak at M1 – 44
THEN The structure is one of the aldehydes

# Knowledge Representation

- Efficiency vs. Comprehensibility
  Additivity
  Modifiability

- Level of representation

# Efficiency and …

| | |
|---|---|
| If | high peak at 57 and high peak at 113 |
| Then | ketone |
| | |
| If | high peak at 57 and high peak at 98 |
| Then | ether |
| | |
| If | high peak at 57 |
| Then | if high peak at 113 then ketone |
| Else | if high peak at 98 then ether |

# Level of Representation

IF

There are peaks at M1 and M2 such that

M1 + M2 = MW + 28 and

M1 is high and M2 is high

THEN

The structure is one of the ketones

# Representation Punchline

Lesson:

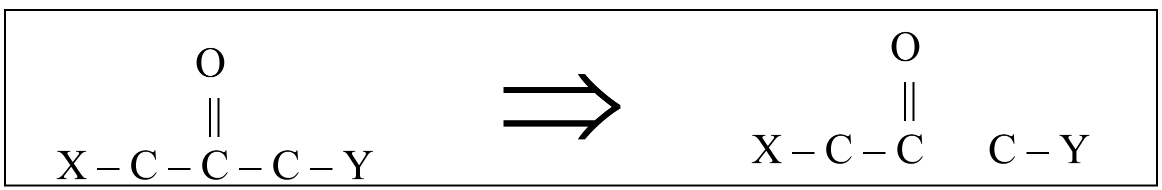
Use the

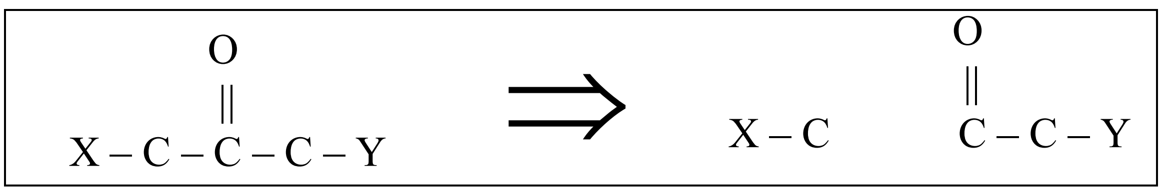
*Highest level*

*Most Transparent*

*Easily modified*

representation you can find





# In the Knowledge Lies the Power

- Lesson:
  Knowledge can obviate the need for search.
  (If you know where to look you don’t have to search)

- Lesson
  Knowledge migrated from the tester to the generator.
  (It’s often better to have a smart generator)

# Building the Program Advances The Field

- The SAINT, SIN, MACSYMA, Risch progression
- Dendral's accumulation, rationalization and development of chemistry knowledge.