# Total Functions for Automated Reasoning

## Building Terminating Theorem Provers

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# Agenda

1. AI & automated reasoning
2. Total programming
3. Unification
4. SAT & DPLL
5. Iterative DPLL

As you can guess/deduce from the title, this is a talk about combining *two topics* I've been working on for the past couple of years.

# Agenda

1. **AI & automated reasoning**
2. **Total programming**
3. Unification
4. SAT & DPLL
5. Iterative DPLL

# Part 1

## *The domain:*

AI & Automated Reasoning

# AI through time

AI is somewhat like "teenage music"

For every decade, it could mean something different:

- 1960s - The Beatles & Expert systems
- 1990s - Backstreet Boys & Spam filter/recommenders
- 2020s - Ariana Grande & Large Language Models

Let us go back to the basics!

# Classic AI tasks

Formulated back in 1950s as "human-level activities performed by computer:"

- Machine translation and text comprehension
- Speech and pattern recognition
- Game playing (chess, checkers, Go, etc)
- *Theorem proving*

We'll focus on the last one:

Here, symbolic (rather than statistical) methods are typically used, and precise guarantees matter the most.

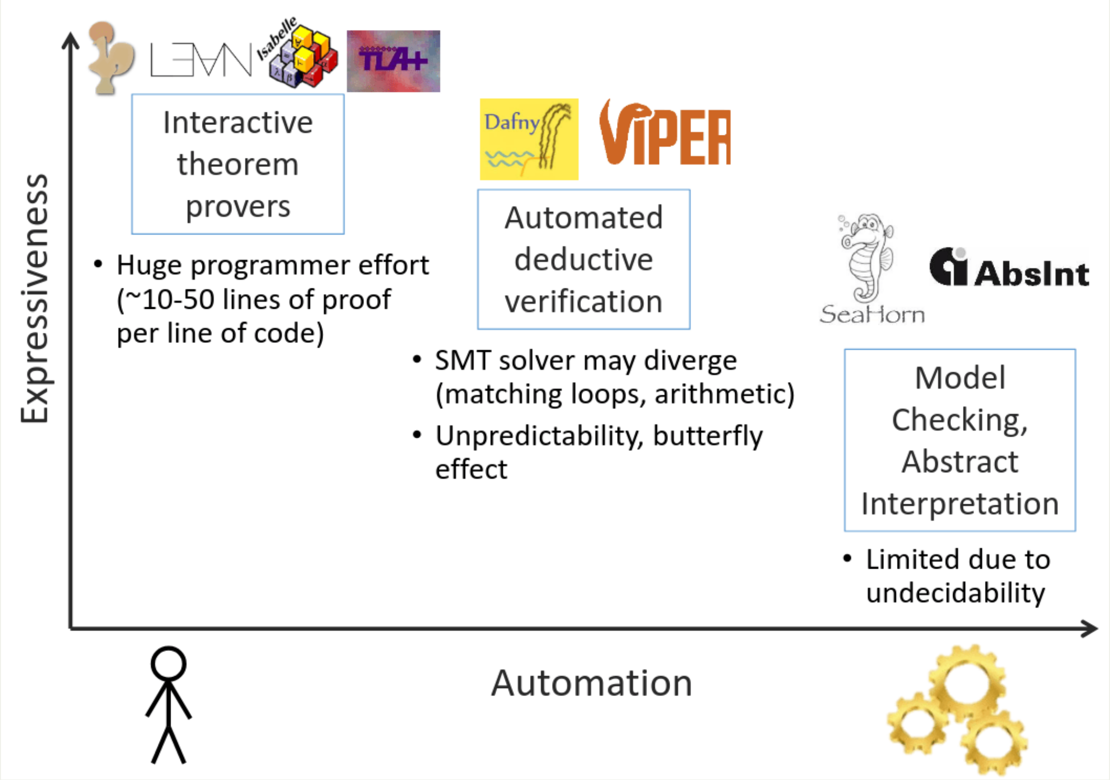
# Theorem proving landscape

- SAT/SMT solvers (Z3/cvc5)
- Computer algebra systems (Mathematica, MAPLE)
- Automated provers (Vampire, E, iProver)
- Logic programming languages (Prolog, λProlog, Datalog)
- Proof assistants (HOL, Coq, Agda, Lean)

There's a struggle between the power of the system and automation.

More versatile systems converge toward general-purpose programming languages.

# Automation vs power




*Shoham, [2019] "Verification of Distributed Protocols Using Decidable Logic"*

We'll use an interactive tool (Agda) to build and verify some simple automated ones.

# Automated reasoning

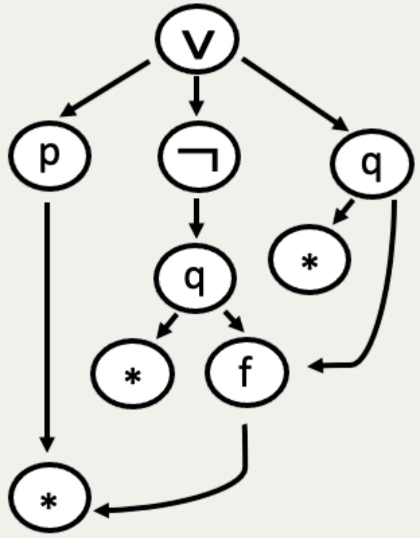
The subfield of symbolic AI focused on theorem proving is referred to as "automated reasoning."

Typically involves:

- operating on syntax with variables
- synthesizing terms/proofs/refutations *(not always)*
- computing finite representations of functions (maps)

The algorithms we'll see use first-order syntax:

no binders (like λ) inside terms.



# Variables and contexts

An important notion when reasoning about variables: *context*

This is what logicians/type theorists write as capital Greek letters ($\Gamma/\Delta$).

A finite set of all variables in the expression.

An overapproximation - can include extra variables not in the term!

We'll use a special (quotient) type `Ctx` for sets of variables (the order and multiplicity in it don't matter).

Has the usual set operators and predicates: $\in$, `union`, `rem`, `minus`

# Part 2

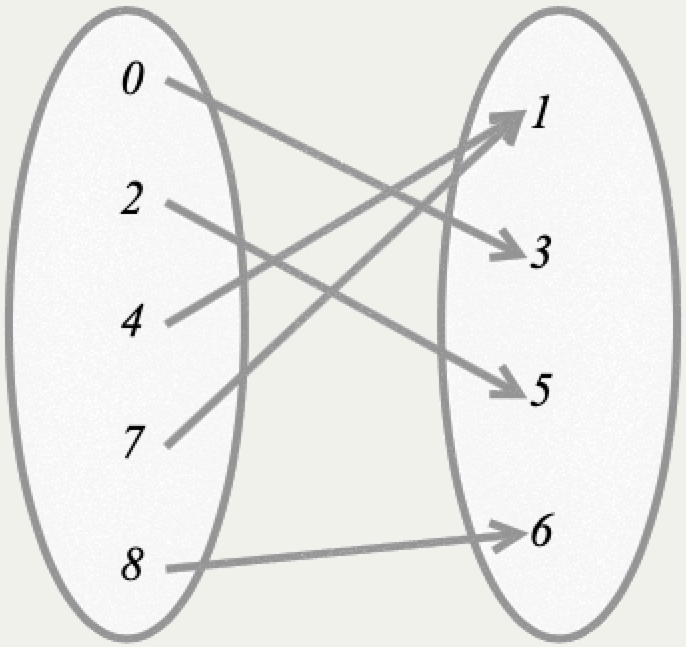
## *The technique:*

Total programming

# The nature of functions

We're going to compute maps/functions, but can we be precise about them?

> *a function from a set X to a set Y assigns to each element of X exactly one element of Y*




(Pure) functions in FP are close to the mathematical definition of a function.

But how do we guarantee the "each" and "exactly one" part?

# Computational functions

Two problems beyond purity:

- not every X is assigned a Y
- a Y is never produced

```haskell
head :: [a] -> a
head []     = error "oops"
head (x:_) = x
```

```haskell
loop :: a -> a
loop x = loop x
```

# Termination matters

Can be costly in critical systems, we typically expect each request/component to finish, even if the system is interactive

> *916 such CVE's between 2000 and 2022*

"Large-scale analysis of non-termination bugs in real-world OSS projects" (2022)

For reasoning algorithms, this means we always get an answer (though it may take a long time).

# Total programming

We can only write programs which:

- cover all inputs
- terminate

The *first* part is relatively trivial (though often requires restructuring your program),

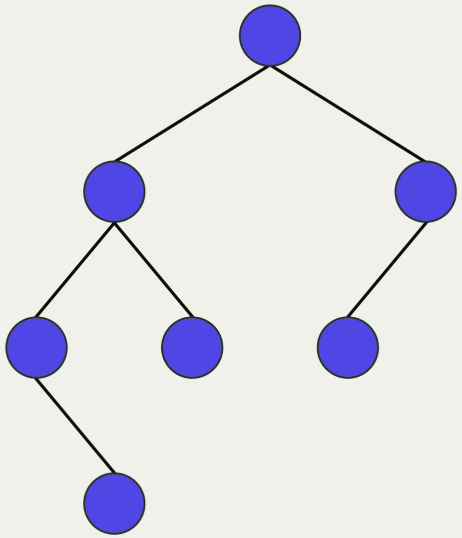
however the *second* involves recursion :(

# Structural recursion

Programs which "consume" syntactically smaller pieces of input:

```
data Tree : 𝒰 where
  leaf : Tree
  node : Tree → Tree → Tree

depth : Tree → ℕ
depth leaf          = 0
depth (node l r)    = 1 + max (depth l) (depth r)
```



# Beyond structural

Here's a simple example that doesn't fit this pattern:

Euclid's GCD algorithm

```
{-# TERMINATING #-}
gcd : ℕ → ℕ → ℕ
gcd n m =
  if m == 0
    then n
    else gcd m (n % m)
```

```
gcd(105, 30) → 105%30 = 15
gcd(30, 15) → 30%15 = 0
gcd(15, 0) = 15
```

We know `n % m < m` but this is not structural!

# Well-founded recursion

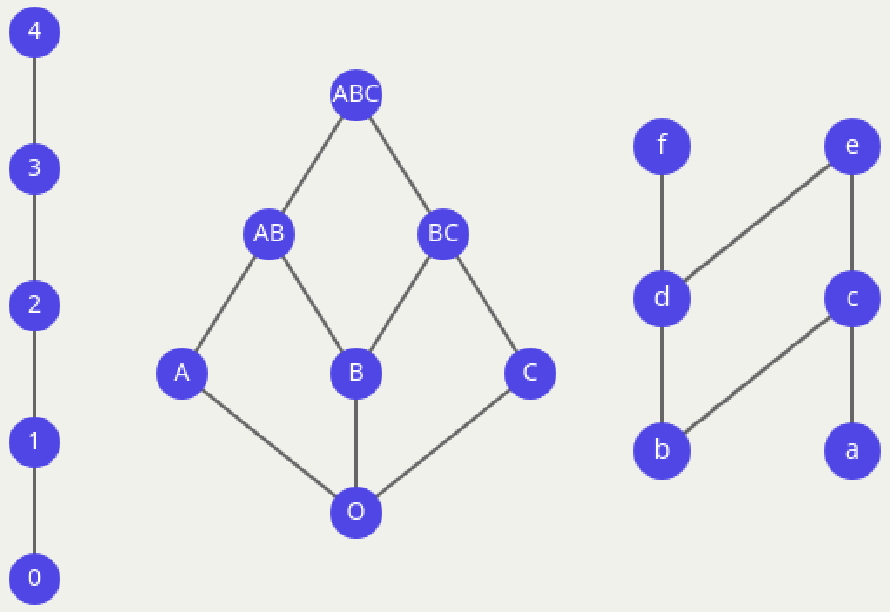
We have to introduce a "measure" that decreases on a type T according to a *well-founded* order.

If you come up with any sequence `... < tx < ty < tz < ...`, it cannot decrease forever

A canonical type with such an order is $(\mathbb{N}, <)$.

Any sequence will eventually end with 0.

Called a linear order, but orders can be branching.



# Well-founded language

Let's introduce a special type for this goal:

```
record □_ (A : T → 𝒰) (x : T) : 𝒰 where
  field call : (x : T) → y < x → A y

-----------------

fix : (A : T → 𝒰)
    → ({t : T} → □ A t → A t)
    → ({t : T} → A t)

-- a non-total fixpoint would be
-- fix : (A → A) → A
```

□A means "A can only be called with an argument smaller than its index"

If the order is well-founded, we can implement the fixed-point combinator!

# Well-founded language - sugar

```
-- implicit
fix : (A : T → 𝒰)
    → ({t : T} → □ A t → A t)
    → ({t : T} → A t)

-- sugar!
fix : (A : T → 𝒰)
    → ∀[ □ A ⇒ A ]
    → ∀[ A ]
```

```
-- explicit
fix : (A : T → 𝒰)
    → ((t : T) → □ A t → A t)
    → ((t : T) → A t)

-- sugar!
fix : (A : T → 𝒰)
    → Π[ □ A ⇒ A ]
    → Π[ A ]
```

Sometimes we want to hide the decreasing argument (make it implicit), other times it's crucial to computation.

# Well-founded GCD

Here's an example of computing a GCD function like this (uses the explicit form):

```
gcd-ty : ℕ → 𝒰
gcd-ty x = (y : ℕ) → y < x → ℕ

gcd-loop : Π[ □ gcd-ty ⇒ gcd-ty ]
gcd-loop x rec y y<x =
  caseᵈ y ≟ 0 of
    λ where
        (yes y=0) → x
        (no y≠0) →
          rec .call
  -- it is safe to do the recursive call
            y<x (x % y)
  -- remainder is smaller
            (%-r-< x y
              (≱→< $ contra ≤0→=0 y≠0))
```

To kick-start the computation, we just need to decide which argument goes first:

```
gcd< : Π[ gcd-ty ]
gcd< = fix gcd-ty gcd-loop

gcd : ℕ → ℕ → ℕ
gcd x y =
  caseᵗ x >=< y of
    λ where
        (LT x<y) → gcd< y x x<y
        (EQ x=y) → x
        (GT y<x) → gcd< x y y<x
```

# Part 3

## *The tutorial level:*

Unification

# Unification

Sometimes called "a Swiss army knife operator".

A family of (semi)algorithms for solving equations.

Match a pattern with gaps in it against data to fill the gaps.

Many applications:

- logic programming
- type inference
- 1st order logic provers
- program synthesis
- ...

# Most General Unifier

First-order MGU: a classical form described in Pierce's TAPL.

Given a pair of terms (or generally a list of pairs),
find a substitution that makes all of them equal (or fail):

```
A       ≟ A       {}
A       ≟ B          FAIL
A       ≟ x       { x ↦ A }
A       ≟ B ⊗ C     FAIL
x       ≟ B ⊗ C   { x ↦ B ⊗ C }
x ⊗ B   ≟ A ⊗ y   { x ↦ A , y ↦ B }
x       ≟ x ⊗ x     FAIL
[ x     ≟ y
, y     ≟ A ]     { x ↦ A , y ↦ A }
```

# Terms & constraints

- Terms are just binary trees with two kinds of leaves
- Variables are an abstract type with equality (think ℕ/String)
- Constraints are pairs of terms

We need both internal and external substitution

```
data Term : 𝒰 where
  ``_ : Var → Term
  _⊗_ : Term → Term → Term
  sy  : String → Term

-- x ⊗ B
example : Term
example = `` x ⊗ sy "B"

Constr : 𝒰
Constr = Term × Term
```

```
-- internal
sub1 : Var → Term → Term → Term
sub1 v t (`` x)  =
  if v == x then t else `` x
sub1 v t (p ⊗ q) =
  sub1 v t p ⊗ sub1 v t q
sub1 v t (sy s) =
  sy s

subs1 : Var → Term → List Constr → List Constr

-- external
Sub : 𝒰
Sub = Map Var Term
```

# Unification code

```
unify : List Constr → Maybe Subst
unify []              = just emptyM
unify ((tl, tr) ∷ cs) =
  if tl == tr
     then unify cs
     else unifyHead tl tr cs

unifyHead : Term → Term
          → List Constr → Maybe Subst
unifyHead (`` v)      tr        cs =
  if occurs v tr then nothing
    else map (insertM v tr) $
         unify (subs1 v tr cs)
unifyHead  tl         (`` v)    cs =
  ... -- symmetrical
unifyHead (lx ⊗ ly) (rx ⊗ ry) cs =
  unify ((lx , rx) ∷ (ly , ry) ∷ cs)     -- adds constraints!
unifyHead _          _          _  =
  nothing
```

# Why does it terminate?

- Can't just count constraints - they increase for the ⊗ case
- Option 1: context size (count variables) - substitution *removes* variables, however the context size **stays the same** for ⊗
- Option 2: count total term size in constraints - *decreases* for ⊗ (one level gets dismantled), but can **grow** for var case

```
tm-size : Term → ℕ
tm-size (p ⊗ q) = 1 + tm-size p + tm-size q
tm-size _       = 1

tm-sizes : List Constr → ℕ
```

Solution: combine 1 and 2!

# Lexicographic order

We can combine two (or generally N) well-founded orders:

```
(a,b) < (x,y) := a < x OR (a = x AND b < y)
```

One component always decreases!

For unification this means:

- Either context decreases (var case),
- Or it stays the same but the total term size does ( + case)

```
Input : 𝒰
Input = Ctx × List Constr

wf-tm : Ctx → Term → 𝒰
wf-tm c t = vars t ⊆ c

wf-input : Input → 𝒰
-- each term in the constraint
-- list is WF
```

```
unify-ty : ℕ × ℕ → 𝒰
unify-ty (x , y) =
    (inp : Input)
  → wf-input inp
  → x = size (inp .fst)
  → y = term-sizes (inp .snd)
  → Maybe Sub
```

# Terminating case for ⊗

```
-- before
unifyHead (lx ⊗ ly) (rx ⊗ ry) cs =
  unify ((lx , rx) ∷ (ly , ry) ∷ cs)

-- after
unify-head-loop rec (ctx , cs) wf (lx ⊗ ly) (rx ⊗ ry) wl wr ex ey =
  rec .call prf-<
     (ctx , ls') prf-wf
     refl refl
  where
  cs' : List Constr
  cs' = (lx , rx) ∷ (ly , ry) ∷ cs
  prf-< : (size ctx , term-sizes cs') < (size ctx , term-sizes cs)
  prf-< = ...
  prf-wf : wf-input (ctx , cs')
  prf-wf = ...
```

# Part 4

## *The main quest:*

SAT & DPLL

# The SAT problem

Classical constraint satisfaction task:

Given a boolean formula with variables,

find an assignment of variables that makes it true (or fail).

Compared to unification:

- we restrict the range of variables (only True/False)
- but we add a semantical constraint (Boolean evaluation)

# The SAT problem examples

```
-- tautologies (true for every assignment)

True
P ∧ Q ⇒ P ∨ Q
((P ⇒ Q) ⇒ P) ⇒ P  -- aka Peirce's law

-- satisfiable (there is an assignment)

P ∧ Q ⇒ Q ∧ R          -- P = Q = True, R = False
                        -- simplifes to True ⇒ False

-- unsatisfiable

P ∧ ¬P
```

# Exponential search

- The most widely used approach is backtracking search
- Naively we can try each variable and flip a previous choice when getting `False`
- However that's $2^n$ operations where n = #variables
- Can we do better?

Generally, in the worst case, **no**! :(

Cook–Levin theorem (1971): SAT is NP-complete

(btw, this is the birth of NP-completeness concept).

But some *heuristics* can make less-than-worst cases tractable.

# DPLL

**Davis–Putnam–Logemann–Loveland algorithm**, 1961

- Still fundamentally performs backtracking search
- But uses 3 heuristics to prune the search substantially
- These are *unit propagation*, *pure literal rule* and *literal selection*

# CNF

DPLL and similar algorithms assume the input is in a *conjunctive normal form*: a big conjunction of disjunctions of possibly negated literals (*clauses*)

```
  ( A ∨ ¬B)
∧ (¬C ∨  D ∨ E)
∧ ...
```

We can always transform into one thanks to boolean reasoning principles (i.e. DeMorgan rule: `¬(P ∨ Q) = ¬P ∧ ¬Q`)

```
True                ~   ∅
False               ~   ()
P ∨ Q               ~   (P ∨ Q)
P ∧ Q               ~   (P) ∧ (Q)
P ∧ Q ⇒ Q ∧ R       ~   (¬P ∨ ¬Q ∨ R)
```

# CNF encoding

Unlike in unification, we push the well-formedness constraint into the literals:

```
data Lit (Γ : Ctx) : 𝒰 where
  Pos : (v : Var) → v ∈ Γ → Lit Γ
  Neg : (v : Var) → v ∈ Γ → Lit Γ

var : Lit Γ → Var
var (Pos v _) = v
var (Neg v _) = v

positive : Lit Γ → Bool
positive (Pos _ _) = true
positive  _        = false
```

```
Clause : Ctx → 𝒰
Clause Γ = List (Lit Γ)

CNF : Ctx → 𝒰
CNF Γ = List (Clause Γ)

literals : CNF Γ → List (Lit Γ)
literals = nub ∘ concat
```

# Unit propagation aka 1-literal rule

Heuristic 1: If a clause consists of a single literal, it must be true, propagate it through the formula

```
unit-clause : CNF Γ → Maybe (Lit Γ)
unit-clause  []                   = nothing
unit-clause (         []  :: c) = unit-clause c
unit-clause ((x ::    []) :: c) = just x
unit-clause ((_ :: _ :: _) :: c) = unit-clause c

unit-propagate : (l : Lit Γ) → CNF Γ → CNF (rem (var l) Γ)
unit-propagate l []        = []
unit-propagate l (f :: c) =
  if has l f
    then unit-propagate l c
    else delete-var (var l) f :: unit-propagate l c

one-lit-rule : CNF Γ → Maybe (Σ[ l : Lit Γ ] (CNF (rem (var l) Γ)))
one-lit-rule cnf =
  map (λ l → l , unit-propagate l cnf) $
  unit-clause cnf
```

# Pure literal rule

Heuristic 2 (aka affirmative-negative rule):

The idea is to delete every literal that occurs strictly positively or strictly negatively (purely)

```
pure-literal-rule :
    (c : CNF Γ)
  → (Σ[ purelits : List (Lit Γ) ]
      (let vs = map var purelits in
      (vs ⊆ Γ) × CNF (minus Γ vs)))
  ⊎ (∀ {l} → l ∈ literals c → negate l ∈ literals c)
...
```

# Literal selection

The previous two rules try to eliminate guessing as much as possible, but eventually, we're going to have to guess a value.

This is where backtracking still happens.

The splitting rule guarantees a result after the pure literal one.

```
posneg-count : CNF Γ → Lit Γ → ℕ
posneg-count cls l =
  let m = count (has          l) cls
      n = count (has $ negate l) cls
    in
  m + n

splitting-rule : (c : CNF Γ)
               → Any positive (literals c)
               → Lit Γ
```

# Putting it all together

```
type Answer = Map Var Bool

dpll-loop : (CNF Γ → Maybe Answer)
          → CNF Γ → Maybe Answer
dpll-loop rec cnf =
  if null? cnf then just emptyM        -- trivially true
    else if has [] cnf then nothing    -- trivially false
      else
        maybe
          (maybe
            (let l = splitting-rule cls in
             map (either (insertLit l)
                         (insertLit (negate l))) $
                 rec (unit-propagate l cnf)
             <+> rec (unit-propagate (negate l) cnf))
            (λ (ls , c) → map (insertLits ls) $ rec c)
            (pure-literal-rule cnf))
          (λ (l , c) → map (insertLit l) $ rec c)
          (one-lit-rule cnf)
```

# Why does this terminate?

Context always decreases:

- For unit propagation by 1
- For pure literal by some n ≥ 1
- For recursive call by 1

This is actually simpler than unification!

We don't need the lexicographic pair, just a single number:

```
DPLL-ty : ℕ → 𝒰
DPLL-ty x =
    {Γ : Ctx}
  → x ≡ size Γ
  → CNF Γ → Maybe Answer
```

# Part 5

## *The boss fight:*

Iterative DPLL

# Iterative DPLL

- Again, the core of the algorithm is backtracking search
- However, the backtracking information is kept on the system stack
  - no tail recursion
- Actual implementations work tail-recursively (iteratively)

```
...
  (map (either (insertLit l)
               (insertLit (negate l))) $
       rec (unit-propagate l cls)
   <+> rec (unit-propagate (negate l) cls))
...
```

# Trail blazing

- We make the stack a first-class object, usually called a *trail*
- Need add a flag do determine if the literal is guessed, which then serves as a backtrack point

```
data Flag : 𝒰 where
  guessed deduced : Flag

Trail : Ctx → 𝒰
Trail Γ = List (Lit Γ × Flag)

trail-lits : Trail Γ → List (Lit Γ)
trail-lits = map fst

trail→answer : Trail Γ → Answer
trail→answer =
  fold-r emp λ (l , _) → upd (var l) (positive l)
```

# Heuristics redux

We get rid of the pure literal rule but perform unit propagation in batches:

```
unit-subpropagate-loop : (CNF Γ → Trail Γ → CNF Γ × Trail Γ)
                       →  CNF Γ → Trail Γ → CNF Γ × Trail Γ
unit-subpropagate-loop rec cnf tr =
  let cnf' = map (filter (not ∘ trail-has tr ∘ negate)) cnf
      newunits = literals (filter (is-fresh-unit-clause tr) cnf')
    in
  if null newunits
    then (cnf' , tr)
    else loop cnf' (map (λ l -> l , deduced) newunits ++ tr)
```

# Iterative DPLL loop

Then we either run into an inconsistency and have to backtrack

```
backtrack : Trail Γ → Maybe (Lit Γ × Trail Γ)
backtrack []                        = nothing
backtrack ((_ , deduced) :: ts) = backtrack ts
backtrack ((p , guessed) :: ts) = just (p , ts)

dpli-loop : CNF Γ
         → (Trail Γ → Maybe Answer)
         →  Trail Γ → Maybe Answer
dpli-loop cnf rec tr =
  let (cnf' , tr') = unit-subpropagate cnf tr in
  if has [] cnf' then                  -- reached False
      maybe
        nothing
        (λ (p , trb) → rec ((negate p , deduced) :: trb))
        (backtrack tr)
    else
      ...
```

# Iterative DPLL loop

Or we have to make a choice:

```
dpli-loop : CNF Γ
          → (Trail Γ → Maybe Answer)
          →  Trail Γ → Maybe Answer
dpli-loop cnf rec tr =
  let (cnf' , tr') = unit-subpropagate cnf tr in
  if has [] cnf' then
      ...
    else                    -- need to guess
      let ps = unassigned cls tr' in
      if null ps
        then just (trail→answer tr')
        else rec ((splitting-rule' cls ps , guessed) :: tr)
```

# Why does any of this terminate?

For unit propagation, the measure is the count of literals still unused in the trail:
(x2 because of polarity)

```
y = 2 · size□ Γ ∸ length tr
```

However this, only works when the trail is *unique* (invariant #1)

# Main loop termination

For the guess case, the unused trail literals also work:

```
rec ((splitting-rule' cls ps , guessed) :: tr)
```

We take the old trail and add a new literal onto it, exhausting unused ones.

But what about the backtracking case?

```
rec ((negate p , deduced) :: trb)
```

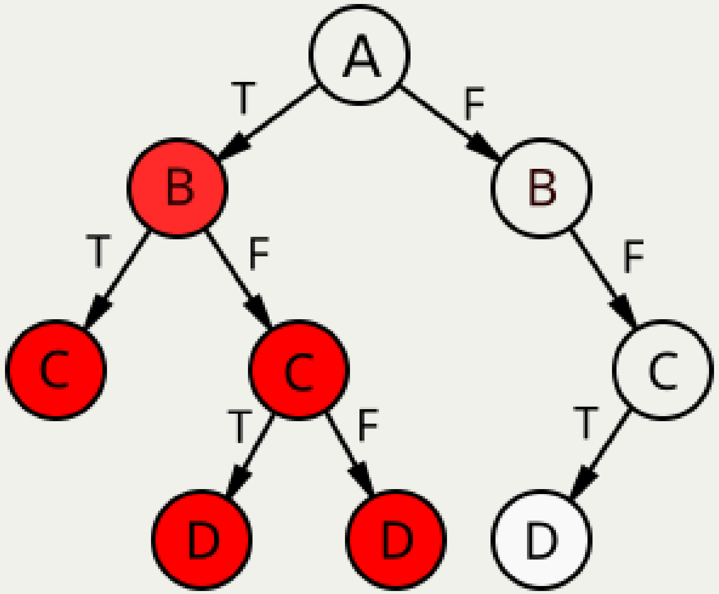
Here `trb` is a suffix of the old trail - it shrinks!

We had the same situation in unification: two kinds of recursive calls, one decreases a measure, the other one increases.

Looks like we need to use the lexicographic product again, but with what?

# Main loop termination - idea

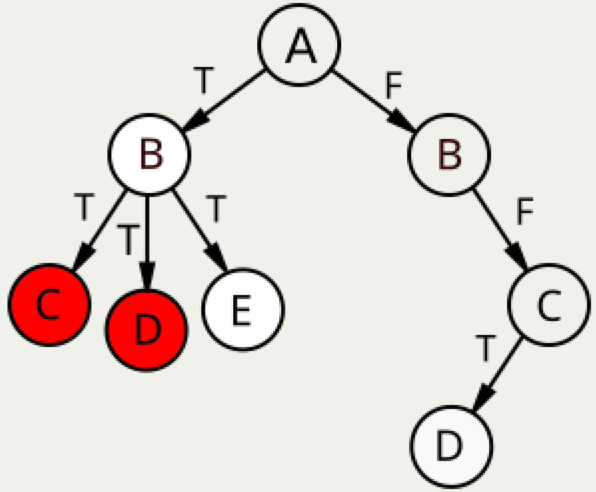
- Intuitively, it's the search space that decreases for backtracking
- But the search tree is generated on the fly
- We need to find a proxy




If we look closely at this tree, we notice that
we never return to discarded branches.
So what sticks around is *discarded literals*.

# Main loop termination - measure

- However, we can't lump them all together - the deduced literals get discarded after backtracking.
- We need to keep a vector of these discarded sets.
- The first part of the measure then is a vector of counts of still-available literals.


The full measure is then a lexicographic product of a vector (N-ary product) of non-discarded assignments corresponding to the guessed level and the number of unused variables in the trace!

*(whew)*

# DPLI termination invariants

For all of this to work, we need the old trail uniqueness invariant and a new one:

1. Variable + polarity should not repeat
2. If a guessed variable is in the trail, its negation doesn't appear before it

The rejected vector/stack also needs an invariant:

If a variable is on level n, its negation appears in the trail after dropping first n guessed variables.

```
Uniq (trail-lits tr) ×
  (∀ x → (x , guessed) ∈ tr
       → negate x ∉ tail-of x (trail-lits tr))

∀ x (f : Fin (size Γ))
   → x ∈ lookup rj f
   → negate x ∈ (trail-lits $ drop-guessed tr (count-guessed tr ∸ fin→ℕ f))
```

Just need to prove that all of these are preserved :/

# DPLI termination type

```
DPLI-ty : {Γ : Ctx} → Vec ℕ (size Γ) × ℕ → 𝒰
DPLI-ty {Γ} (x , y) =
    (tr : Trail Γ)
  → Trail-invariant tr
  → (rj : Rejectstack Γ)
  → Rejectstack-invariant rj tr
  → x ≡ map (λ q → 2 · size Γ ∸ size q) rj
  → y ≡ 2 · size Γ ∸ length tr
  → Maybe Answer
```

# Conclusion

# Lessons learned

- Writing out termination proofs forces you to understand how the algorithm actually works, in the form of its invariants.
- Control flow tricks make termination harder :(
- Once you determine the invariants, you have more freedom to restructure your algorithm, make it more modular, experiment with different representations, and so on.

# Lessons learned

- More generally, from a mathematical point of view, automated reasoning is about syntax, finite sets, maps, and intricate order relations.
- And order theory is just a cut-down version of category theory, but that is a story for another time…

# References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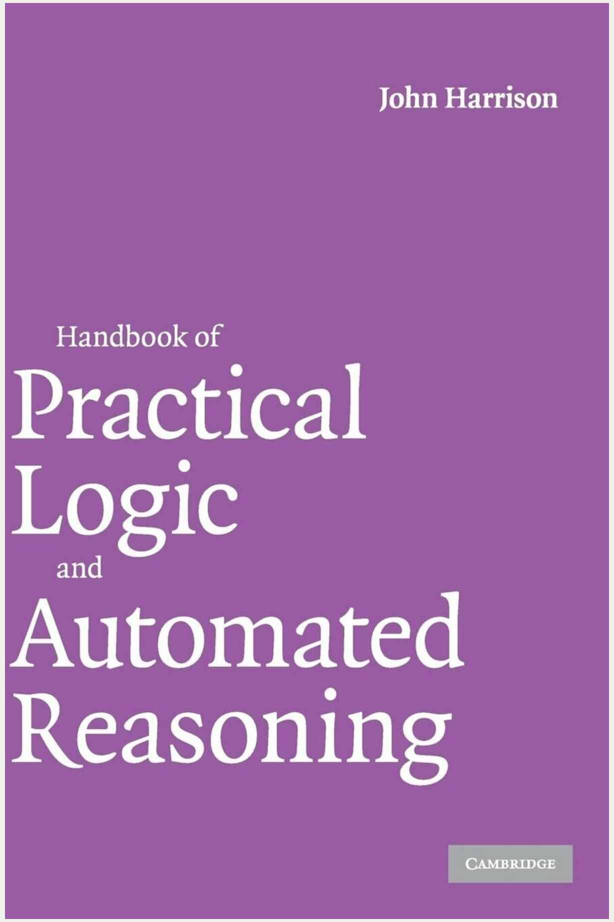

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https://github.com/clayrat/lw25-talk

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