Lecture outline

1. Validity Checking in Propositional Logic
   - General Remarks
   - Normal Forms
   - Validity/Satisfiability in CNFs
   - SAT solvers

2. Validity in First-Order Logic
   - General Remarks
   - Normal Forms
   - Herbrand’s Theorem and Semi-Decidability
   - Decidable Fragments

3. Validity in First-Order Theories
   - Basic Concepts
   - Some Theories
   - SMT Provers
Given a propositional formula $A$, there are two obvious decision problems regarding its validity status:

**Validity problem (VAL):** Given a formula $A$, is $A$ valid?

**Satisfiability problem (SAT):** Given a formula $A$, is $A$ satisfiable?

Recall:

- $A$ is valid if $\mathcal{M} \models A$ for every model (valuation) $\mathcal{M}$;
- $A$ is satisfiable if $\mathcal{M} \models A$ for some model $\mathcal{M}$.
- Hence, $A$ is valid iff $\neg A$ is not satisfiable.

Two conceivable approaches to settle these problems:

- **Semantic method** – directly using the definition of validity;
- **Deductive method** – exploit *soundness* and *completeness* theorems.
Truth-Tables

- Only propositional symbols used in a formula play a role in its validity.

\[
\begin{array}{|c|c|c|c|}
\hline
A & B & ((A \rightarrow B) \rightarrow A) & \rightarrow A \\
\hline
F & F & T & F & T \\
F & T & T & F & T \\
T & F & F & T & T \\
T & T & T & T & T \\
\hline
\end{array}
\]

- *truth-tables* can be used to decide both VAL and SAT
- \(2^n\) entries (\(n\) the number of propositional symbols)
- unfeasible for moderately big formulas
- is it possible to devise better decision procedures?

The structure of logical validity allows for much better algorithms.

Strategy for tackling these problems:

1. one first preprocesses the input formula to a restricted syntactic class, preserving the property under evaluation (validity for VAL, and satisfiability for SAT)
2. an efficient method is then applied to check the validity of formulas in this restricted class

both steps should be kept “reasonably effective” since they are intended to be run in sequence
SAT and VAL are indeed difficult problems

Both problems play a distinctive role in the hierarchy of complexity classes:

- SAT is a *NP-complete* problem, i.e. any problem in NP is reducible in polynomial-time to SAT;
- VAL is a *coNP-complete* problem.

Hence, it is believed that both SAT and VAL cannot be solved in polynomial-time.

*If a polynomial-time algorithm to solve SAT or VAL were ever found, this would settle the P = NP question*

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**Normal Forms**

- *Normal forms* are syntactical classes of formulas (i.e. formulas with a restricted “shape”)
- ...that can be considered to be representative of the whole set of formulas.
- The idea is that we associate to a normal form a *normalization procedure* that, for any formula, computes a formula of this restricted class that is *equivalent* (or *equisatisfiable*) with the original.
Negation Normal Form

Definition
A propositional formula $A$, we say that it is in *negation normal form (NNF)*, if
the implication connective is not used in $A$, and negation is only applied to
atomic formulas (propositional symbols or $\bot$);

- Propositional symbols or their negation are called *literals*
- Hence, a formula in NNF is a formula built up from literals, constants $\bot$ and $\top$ (i.e. $\neg\bot$), disjunctions and conjunctions.
- For every formula $A$, it is always possible to find an equivalent formula $B$ in NNF ($B$ is called a NNF of $A$).
- Normalisation procedure: repeatedly replace any subformula that is an instance of the left-hand-side of one of the following equivalences by the corresponding right-hand-side.
  
  $A \rightarrow B \equiv \neg A \lor B \quad \neg A \equiv A$
  $\neg (A \land B) \equiv \neg A \lor \neg B \quad \neg (A \lor B) \equiv \neg A \land \neg B$

- Complexity of the normalisation procedure: linear on the size of formula.

Conjunctive/Disjunctive Normal Form

Definition
Given a propositional formula $A$, we say that it is in:

- *Conjunctive Normal Form (CNF)* if it is a conjunction of disjunctions of literals, i.e. $A = \bigwedge_i \bigvee_j l_{ij}$, for literals $l_{ij}$;
- *Disjunctive Normal Form (DNF)* if it is a disjunction of conjunctions of literals, i.e. $A = \bigvee_i \bigwedge_j l_{ij}$, for literals $l_{ij}$,

where $\bot$ (resp. $\top$) is considered to be the empty disjunction (resp. the empty conjunction). The inner conjunctions/disjunctions are called *clauses*.

- CNFs and DNFs are dual concepts. We will restrict attention to CNFs.
- Normalisation Procedure: to a formula already in NNF apply, the following equivalences (left-to-right):

  $A \lor (B \land C) \equiv (A \lor B) \land (A \lor C) \quad (A \land B) \lor C \equiv (A \lor C) \land (B \lor C)$
  $A \land \bot \equiv \bot \quad \bot \land A \equiv \bot \quad A \land \top \equiv A \quad \top \land A \equiv A$
  $A \lor \bot \equiv A \quad \bot \lor A \equiv A \quad A \lor \top \equiv \top \quad \top \lor A \equiv \top$
Let us compute the CNF of \(((P \rightarrow Q) \rightarrow P) \rightarrow P\). The first step is to compute its NNF by transforming implications into disjunctions and pushing negations to proposition symbols:

\[
((P \rightarrow Q) \rightarrow P) \rightarrow P \equiv \neg((P \rightarrow Q) \rightarrow P) \lor P \\
\equiv \neg(\neg(P \lor Q) \lor P) \lor P \\
\equiv \neg(\neg(P \lor Q) \lor P) \lor P \\
\equiv (\neg(P \lor Q) \land \neg P) \lor P \\
\equiv ((\neg P \lor Q) \land \neg P) \lor P
\]

To reach a CNF, distributivity is then applied to pull the conjunction outside:

\[
((\neg P \lor Q) \land \neg P) \lor P \equiv (\neg P \lor Q \lor P) \land (\neg P \lor P).
\]

- The CNF translation has an exponential worst-case running time
  - distributive equivalences duplicate formulas...
  - ...the resulting formula can thus be exponentially bigger than the original formula.
- The following formula illustrates this bad behaviour:

\[
(P_1 \land Q_1) \lor (P_2 \land Q_2) \lor \ldots \lor (P_n \land Q_n) \\
\equiv (P_1 \lor (P_2 \land Q_2) \lor \ldots \lor (P_n \land Q_n)) \land (Q_1 \lor (P_2 \land Q_2) \lor \ldots \lor (P_n \land Q_n)) \\
\equiv \ldots \\
\equiv (P_1 \lor \ldots \lor P_n) \land \\
\quad (P_1 \lor \ldots \lor P_{n-1} \lor Q_n) \land \\
\quad (P_1 \lor \ldots \lor P_{n-2} \lor Q_{n-1} \lor P_n) \land \\
\quad (P_1 \lor \ldots \lor P_{n-2} \lor Q_{n-1} \lor Q_n) \land \\
\quad \ldots \land \\
\quad (Q_1 \lor \ldots \lor Q_n)
\]

- The original formula has \(2 \cdot n\) literals,
- while the corresponding CNF has \(2^n\) disjunctive clauses, each with \(n\) literals.
- Conclusion: in practice, it is not reasonable to reduce a formula in its equivalent CNF as part of a VAL procedure.
There are alternative conversions to CNF that avoid this exponential growth.

- instead of producing an equivalent formula, produce formulas that are *equisatisfiable* with the original formula, i.e.

> the resultant formula is satisfiable iff the original formula is

- These alternative conversions compute what is called the *Definitional CNF* of a formula,
- ...because they often rely on the introduction of new proposition symbols that act as names for subformulas of the original formula.

The weaker requirements of *definitional CNF* makes them suitable for solving SAT (not VAL).

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The previous example can be handled by associating a new proposition symbol \( R_i \) to each conjunctive clause \((P_i \land Q_i)\).

New clauses are added to enforce that new proposition symbols are tied with the original conjunctive clauses: \( (\neg R_i \lor P_i) \) and \( (\neg R_i \lor Q_i) \).

The resulting formula is thus:

\[
(R_1 \lor \cdots \lor R_n) \land (\neg R_1 \lor P_1) \land (\neg R_1 \lor Q_1) \land \cdots \land (\neg R_n \lor P_n) \land (\neg R_n \lor Q_n)
\]

Let \( \mathcal{M} \) be any model satisfying this CNF:

- If \( \mathcal{M} \models R_i \) (for some \( i \)), then \( \mathcal{M} \models P_i \) and \( \mathcal{M} \models Q_i \).
- It is then clear that \( \mathcal{M} \) witnesses that the original formula is satisfiable.

The resultant CNF is not significantly bigger than the original formula (but has more propositional symbols).
Validity in CNFs

- Recall that CNFs are formulas with the following shape (each \( l_{ij} \) denotes a literal):
  \[
  (l_{11} \lor l_{12} \lor \ldots \lor l_{1k}) \land \ldots \land (l_{n1} \lor l_{n2} \lor \ldots \lor l_{nj})
  \]
- Associativity, commutativity and idempotence of both disjunction and conjunction allow us to treat each CNF as a set of sets of literals
  \[
  S = \{\{l_{11}, l_{12}, \ldots, l_{1k}\}, \ldots, \{l_{n1}, l_{n2}, \ldots, l_{nj}\}\}
  \]
- An empty inner set (clause) will be identified with \( \bot \), and an empty outer set with \( \top \).
- Simple observations:
  - a CNF is a tautology if and only if all of its clauses are tautologies;
  - If a clause \( c \in S \) is a tautology, it can be removed from \( S \) without affecting its validity status, i.e. \( S \equiv S \setminus \{c\} \);
  - A clause \( c \) is a tautology precisely when there exists a proposition symbol \( P \) such that \( \{P, \neg P\} \subseteq c \). A clause \( c \) such that \( \{P, \neg P\} \subseteq c \) for some \( P \) is said to be closed.
  - A CNF is a tautology if and only if all of its clauses are closed.
- Dually, a DNF is a contradiction if and only if all of its clauses are closed.

Example

- Consider the formula \( A = ((P \to Q) \to P) \to P \) (previous example). Its CNF is
  \[
  \{\{\neg P, Q, P\}, \{\neg P, P\}\}
  \]
  Since all clauses are closed, we conclude that \( A \) is a tautology.
- Consider now \( B = (P \to Q \lor R) \land \neg(P \land Q \to R) \). Its CNF is
  \[
  \{\{\neg A, A, \neg B\}, \{A, \neg B\}\}
  \]
  the clause \( \{A, \neg B\} \) is not closed, hence the formula is not a tautology (i.e. it is refutable).
- However, the applicability of this simple criterion for VAL is compromised by the potential exponential growth in the CNF transformation.
- As explained before, this limitation is overcome considering instead SAT...
- ...with satisfiability preserving CNFs (definitional CNF).
- obs.: The dual criterion can be used to decide (un)SAT on a propositional formula \( A \) (using its equivalent DNF).
One of the most important methods to check satisfiability of CNFs is the \textit{Davis-Putnam-Logemann-Loveland procedure (DPLL)}.

DPLL is an algorithm for verifying if a particular CNF is a contradiction. It incrementally constructs a model compatible with a CNF...

...if no such model exists, the formula is signaled as a contradiction. Otherwise it is satisfiable.

Basic observation: \textit{if we fix the interpretation of a particular proposition symbol, we are able to simplify the corresponding CNF accordingly}

Consider a proposition symbol $P$, a CNF $S$ and a clause $c \in S$. For any model $\mathcal{M}$:
- If $P \in \mathcal{M}$,
  - if $P \in c$ then $\mathcal{M} \models c$. Thus $\mathcal{M} \models S$ iff $\mathcal{M} \models S \setminus \{c\}$. In short, clauses containing $P$ can be ignored.
  - $\mathcal{M} \models c$ iff $\mathcal{M} \models c \setminus \{\neg P\}$. In short, $\neg P$ can be removed from every clause in $S$.
- Analogously if $P \notin \mathcal{M}$ (i.e. $\mathcal{M} \models \neg P$):
  - if $\neg P \in c$ then $\mathcal{M} \models S$ iff $\mathcal{M} \models S \setminus \{c\}$;
  - $\mathcal{M} \models c$ iff $\mathcal{M} \models c \setminus \{P\}$.

These observations can be summarised as follows.

\textbf{Definition}

Let $l$ be a literal and $S$ a CNF.
- The \textit{opposite} of $l$ (denoted by $\neg l$) is defined as
  \[ l = \begin{cases} 
  \neg P & , \text{if } l = P; \\
  P & , \text{if } l = \neg P. 
  \end{cases} \]
- The \textit{split} of $S$ by $l$ is
  \[ \text{split}^l(S) = \{c \setminus \neg l \mid c \in S, l \notin c\} \]

Informally, $\text{split}^l(S)$ is a simplification of $S$ assuming $l$ holds.
- Note that neither $l$ nor $\neg l$ occur in any clause of $\text{split}^l(S)$ or $\text{split}^{\neg l}(S)$.
- For a CNF $S$ and proposition symbol $P$,
  \[ S \equiv (P \rightarrow \text{split}^P(S)) \land (\neg P \rightarrow \text{split}^{\neg P}(S)) \]
Recursively applying this simplification for every symbol occurring in a CNF is the heart of the DPLL algorithm.

**Definition (DPLL Algorithm)**

Let $S$ be a CNF. The DPLL algorithm is defined recursively by

$$
\text{DPLL}(S) = \begin{cases} 
F & \text{if } S = \top \\
T & \text{if } \bot \in S \\
\text{DPLL}(\text{split}(S)) \text{ and } \text{DPLL}(\text{split}(S)) & \text{otherwise}
\end{cases}
$$

where the literal $l$ chosen in the recursive step is any literal appearing in $S$.

- The CNF $S$ is a contradiction if $\text{DPLL}(S) = T$;
- ...and satisfiable otherwise (a model can be extracted from the path of choices performed by the algorithm).

**Example**

- The recursion tree for the execution of DPLL on the CNF $\neg P \lor \neg Q \lor \neg R \land (\neg Q \lor \neg R) \land Q \land R$.

Since all the leaves are tagged with $T$, the formula is a contradiction.
Consider now the recursion tree for \((\neg P \lor \neg Q \lor \neg R) \land (\neg Q \lor \neg R) \land R\).

\[
\begin{align*}
\{\neg P, \neg Q, \neg R\}, \{\neg Q, \neg R\}, \{R\} \\
\{\neg P, \neg Q\}, \{\neg Q\} \\
\{\neg P\}, {} \\
\text{True} \\
\{\neg Q\} \\
\text{split} \\
\{\neg R\} \\
\{\} \\
\text{split} \\
\text{split} \\
\text{True} \\
\text{False}
\end{align*}
\]

A false leaf signals that the formula is satisfiable.

The positive literals that occur in the corresponding path give rise to a model that validates the formula.

The behaviour of the algorithm is highly dependent on the order in which the proposition symbols are chosen.

Particular attention to how the next symbol is selected, in order to maximize the efficiency of the algorithm.

Additional optimisations and heuristics are often explored to avoid unnecessary branches during execution

- **unit-propagation**: singleton clauses \(\{l\} \in S\) can (should) be used to simplify the CNF;
- **pure literals**: literals that occur in clauses of \(S\) always with a given polarity can be removed.

An heuristic often used is to choose the most frequent propositional symbol in \(S\).
Propositional satisfiability has been successfully applied to perform hardware and software verification.

Specialised tools exist that are capable of handling large instances of the satisfiability problem.

A particular class of tools that are close to the computational approach exposed are the so-called SAT solvers.

The *satisfiability library* SATlib\(^1\) is an online resource that proposes, as a standard, a unified notation and a collection of benchmarks for performance evaluation and comparison of tools.

Such a uniform test-bed has been serving as a framework for regular tool competitions organised in the context of the regular SAT conferences.\(^2\)

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\(^1\)http://www.satlib.org/
\(^2\)http://www.satcompetition.org
Unsurprisingly, the problem of determining whether an arbitrary first-order sentence is valid is significantly harder than for the propositional case. In fact, it is impossible to solve this problem in its full generality.

**Theorem**

The validity problem for first-order logic is undecidable.

This negative result (undecidability) is a direct consequence of a positive feature of first-order logic – its expressive power. Moreover, it does not preclude however restricted instances of the general problem from being solvable. We will see that the problem of validity-checking of first-order formulas can, to some extent, be reduced to the propositional case. This requires to restrict the use of quantifiers in formulas.

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**Negation Normal Form**

**Definition**

A first-order formula is in *negation normal form* (NNF) if the implication connective is not used in it, and negation is only applied to atomic formulas.

Every first-order formula is equivalent to a NNF formula. It can be computed by extending the propositional NNF normalisation with specific laws to handle quantifiers.

\[
\phi \rightarrow \psi \equiv \neg \phi \lor \psi \\
\neg (\phi \land \psi) \equiv \neg \phi \lor \neg \psi \\
\neg \forall x. \phi \equiv \exists x. \neg \phi \\
\neg \exists x. \phi \equiv \forall x. \neg \phi
\]

Example: to compute the NNF of \( \forall x. (\forall y. P(x, y) \lor Q(x)) \rightarrow \exists z. P(x, z) \).

\[
\forall x. (\forall y. P(x, y) \lor Q(x)) \rightarrow \exists z. P(x, z) \equiv \\
\forall x. \neg (\forall y. P(x, y) \lor Q(x)) \lor \exists z. P(x, z) \equiv \\
\forall x. \exists y. (\neg P(x, y) \land \neg Q(x)) \lor \exists z. P(x, z)
\]
Prenex Normal Form

- If $x$ does not occur free in $\psi$, then the following equivalences hold.

\[
(\forall x \cdot \phi) \land \psi \equiv \forall x \cdot \phi \land \psi \quad \psi \land (\forall x \cdot \phi) \equiv \forall x \cdot \psi \land \phi
\]

\[
(\forall x \cdot \phi) \lor \psi \equiv \forall x \cdot \phi \lor \psi \quad \psi \lor (\forall x \cdot \phi) \equiv \forall x \cdot \psi \lor \phi
\]

\[
(\exists x \cdot \phi) \land \psi \equiv \exists x \cdot \phi \land \psi \quad \psi \land (\exists x \cdot \phi) \equiv \exists x \cdot \psi \land \phi
\]

\[
(\exists x \cdot \phi) \lor \psi \equiv \exists x \cdot \phi \lor \psi \quad \psi \lor (\exists x \cdot \phi) \equiv \exists x \cdot \psi \lor \phi
\]

- The applicability of these equivalences can always be assured by appropriate renaming of bound variables.

- Applying these equations to a NNF leads to formulas where quantifiers are in the outermost position.

**Definition**

A formula is in **prenex form** if it is of the form $Q_1 x_1 . Q_2 x_2 . . . Q_n x_n . \psi$ where each $Q_i$ is a quantifier (either $\forall$ or $\exists$) and $\psi$ is a quantifier-free formula.

Herbrand/Skolem Normal Form

**Definition (Herbrand and Skolem Forms)**

Let $\phi$ be a first-order formula in prenex normal form. The **Herbrandization** of $\phi$ (written $\phi^H$) is an existential formula obtained from $\phi$ by repeatedly and exhaustively applying the following transformation:

\[
\exists x_1, \ldots, x_n . \forall y . \psi \leadsto \exists x_1, \ldots, x_n . \psi[f(x_1, \ldots, x_n)/y]
\]

with $f$ a fresh function symbol with arity $n$ (i.e. $f$ does not occur in $\psi$).

Dually, the **Skolemization** of $\phi$ (written $\phi^S$) is a universal formula obtained from $\phi$ by repeatedly applying the transformation:

\[
\forall x_1, \ldots, x_n . \exists y . \psi \leadsto \forall x_1, \ldots, x_n . \psi[f(x_1, \ldots, x_n)/y]
\]

again, $f$ is a fresh function symbol with arity $n$.

**Herbrand normal form** (resp. **Skolem normal form**) formulas are those obtained by this process.
Proposition

Let $\phi$ be a first-order formula in prenex normal form. $\phi$ is valid iff its Herbrandization $\phi^H$ is valid. Dually, $\phi$ is unsatisfiable iff its Skolemization $\phi^S$ is unsatisfiable.

- It is convenient to write Herbrand and Skolem formulas using vector notation $\exists \bar{x}. \psi$ and $\forall \bar{x}. \psi$ (with $\psi$ quantifier free), respectively.
- The quantifier-free sub-formula can be furthered normalised:
  - Universal CNF: $\forall \bar{x}. \bigwedge_i \bigvee_j l_{ij}$
  - Existential DNF: $\exists \bar{x}. \bigvee_i \bigwedge_j l_{ij}$
  where literals are either atomic predicates or negation of atomic predicates.
- Herbrandization/Skolemization change the underlying vocabulary. These additional symbols are called Herbrand/Skolem functions.
- (obs: this observation alone suffices to show that a formula and its Herbrandization/Skolemization are not equivalent.)

Herbrand Model

Definition (Herbrand Interpretation)

Let $\mathcal{V}$ be a first-order vocabulary and assume $\mathcal{V}$ has at least one constant symbol (otherwise, we explicitly expand the vocabulary with such a symbol). A Herbrand Interpretation $\mathcal{H} = (D_\mathcal{H}, I_\mathcal{H})$ is a $\mathcal{V}$-structure specified by a set of ground atomic predicates (i.e. atomic predicates applied to ground terms), also denoted by $\mathcal{H}$. The interpretation structure is given as follows:

- Interpretation domain: $D_\mathcal{H}$ is the set of ground terms for the vocabulary $\mathcal{V}$. It is called the Herbrand universe for $\mathcal{V}$.
- Interpretation of constants: for every $c \in \mathcal{V}$, $I_\mathcal{H}(c) = c$;
- Interpretation of functions: for every $f \in \mathcal{V}$ with $\text{ar}(f) = n$, $I_\mathcal{H}(f)$ consists of the $n$-ary function that, given ground terms $t_1, \ldots, t_n$, returns the ground term $f(t_1, \ldots, t_n)$;
- Interpretation of predicates: for every $P \in \mathcal{V}$ with $\text{ar}(P) = n$, $I_\mathcal{H}(P)$ is the $n$-ary relation $\{(t_1, \ldots, t_n) \mid P(t_1, \ldots, t_n) \in \mathcal{H}\}$. 
Herbrand’s Theorem

Lemma

An existential formula \( \phi \) is valid iff for every Herbrand model \( \mathcal{H} \), \( \mathcal{H} \models \phi \). Dually, a universal formula \( \phi \) is unsatisfiable iff there exists no Herbrand model \( \mathcal{H} \) such that \( \mathcal{H} \models \phi \).

Theorem (Herbrand’s Theorem)

An existential first-order formula \( \exists x. \psi \) (with \( \psi \) quantifier-free) is valid iff there exists an integer \( k \) and ground instances \( \psi_{\sigma_1}, \ldots, \psi_{\sigma_k} \) such that \( \psi_{\sigma_1} \lor \cdots \lor \psi_{\sigma_k} \) is propositionally valid.

Dually, a universal formula \( \forall x. \psi \) (with \( \psi \) quantifier-free) is unsatisfiable iff there exists an integer \( k \) and closed instances \( \psi_{\sigma_1}, \ldots, \psi_{\sigma_k} \) such that \( \psi_{\sigma_1} \land \cdots \land \psi_{\sigma_k} \) is propositionally unsatisfiable.

Application

Theorem (Semi-Decidability)

The problem of validity of first-order formulas is semi-decidable, i.e. there exists a procedure that, given a first-order formula, answers “yes” iff the formula is valid (but might not terminate if the formula is not valid).

- An interesting refinement is to investigate fragments in which bounds can be established for searching the ground instance space.
- This immediately leads to a bound on the number of instances whose search is required by Herbrand’s theorem...
- ...turning validity of formulas decidable.
- Clearly if the set of ground terms is finite, the set of ground instances of the formula under scrutiny will be finite as well.
Decidable Fragments

- If the underlying vocabulary has no function symbol, the set of ground terms is finite.
- Note however that function symbols might be introduced during the Herbrandization/Skolemization.
- Restricting attention to formulas whose prenex normal form has the shape

\[ \forall x. \exists y. \psi \]

ensures that only constants are introduced by Herbrandization.
- This fragment of formulas is normally known as the AE fragment, owing its name to the alternation of quantifiers allowed (A refers to the universal quantifier and E to existential quantifier).
- The class of formulas can be further enlarged by observing that a formula not in AE may be equivalent to one in AE (e.g. miniscope — pushing existential quantifiers inside the formula, thus minimizing their scopes).
- Monadic formulas (i.e. formulas containing only unary predicates) are such a class of formulas. Hence, they constitute a decidable fragment of first-order logic.
When judging the validity of first-order formulas we are typically interested in a particular domain of discourse...

... which in addition to a specific underlying vocabulary includes also properties that one expects to hold.

That is, we are often interested in moving away from pure logical validity (i.e. validity in all models) towards a more refined notion of validity restricted to a specific class of models.

A natural way for specifying such a class of models is by providing a set of axioms (sentences that are expected to hold in them).

Alternatively, one can pinpoint the models of interest.

First-order Theories provides the basis for the kind of reasoning just described.

**First-Order Theories**

*Definition*

Let $\mathcal{V}$ be a vocabulary of a first-order language.

- A first-order theory $\mathcal{T}$ is a set of $\mathcal{V}$-sentences that is closed under derivability (i.e., $\mathcal{T} \vdash \phi$ implies $\phi \in \mathcal{T}$). A $\mathcal{T}$-structure is a $\mathcal{V}$-structure that validates every formula of $\mathcal{T}$.

- A formula $\phi$ is $\mathcal{T}$-valid (resp. $\mathcal{T}$-satisfiable) if every (resp. some) $\mathcal{T}$-structure validates $\phi$.

- A first-order theory $\mathcal{T}$ is said to be a consistent theory if at least one $\mathcal{T}$-structure exists. $\mathcal{T}$ is said to be a complete theory if, for every $\mathcal{V}$-sentence $\phi$, either $\mathcal{T} \models \phi$ or $\mathcal{T} \models \neg \phi$. $\mathcal{T}$ is said to be a decidable theory if there exists a decision procedure for checking $\mathcal{T}$-validity.

- Let $\mathcal{K}$ be a class of $\mathcal{V}$-structures. The theory of $\mathcal{K}$, denoted by $\text{Th}(\mathcal{K})$, is the set of sentences valid in all members of $\mathcal{K}$, i.e., $\text{Th}(\mathcal{K}) = \{ \psi \mid \mathcal{M} \models \psi, \text{ for all } \mathcal{M} \in \mathcal{K} \}$. Conversely, given a set of $\mathcal{V}$-sentences $\Gamma$, the class of models for $\Gamma$ is defined as $\text{Mod}(\Gamma) = \{ \mathcal{M} \mid \text{ for all } \phi \in \Gamma, \mathcal{M} \models \phi \}$.

- A subset $\mathcal{A} \subseteq \mathcal{T}$ is called an axiom set for the theory $\mathcal{T}$ when $\mathcal{T}$ is the deductive closure of $\mathcal{A}$, i.e. $\psi \in \mathcal{T}$ iff $\mathcal{A} \vdash \psi$. A theory $\mathcal{T}$ is finitely (resp. recursively) axiomatisable if it possesses a finite (resp. recursive) set of axioms.
Whenever a theory $T$ is axiomatisable (by a finite or recursive set of axioms $\mathcal{A}$), it makes sense to extend the first-order logic proof system $\mathcal{N}_{\text{FOL}}$ with an axiom-schema:

$$\Gamma \vdash \phi \text{ if } \phi \in \mathcal{A}$$

Observe that the requirement that $\mathcal{A}$ be a recursive set is crucial to ensure that the applicability of these axioms can effectively be checked.

Moreover, if a theory $T$ has a recursive set of axioms, the theory itself is recursively enumerable (hence, the $T$-validity problem is semi-decidable).

If $T$ is a complete theory, then any $T$-structure validates exactly the same set of $T$-sentences (the theory itself).

For a given $\mathcal{V}$-structure $\mathcal{M}$, the theory $\text{Th}(\mathcal{M})$ (of a single-element class of $\mathcal{V}$-structures) is complete. These semantically defined theories are useful when one is interested in reasoning in some specific mathematical domain such as the natural numbers, rational numbers, etc.

However, we remark that such theory may lack an axiomatisation, which seriously compromises its use in purely deductive reasoning.

If a theory is complete and has a recursive set of axioms, it can be shown to be decidable.

The decidability criterion for $T$-validity is crucial for mechanised reasoning in the theory $T$.

It may be necessary (or convenient) to restrict the class of formulas under consideration to a suitable fragment;

The $T$-validity problem in a fragment refers to the decision about whether or not $\phi \in T$ when $\phi$ belongs to the fragment under consideration.

A fragment of interest is the fragment consisting of universal formulas, often referred to as the quantifier-free fragment.
### Some Theories

**Equality and Uninterpreted-Functions** $\mathcal{T}_E$: theory whose the only axioms are the ones related with equality (reflexivity and congruence). $\mathcal{T}_E$-validity is undecidable in general, but efficiently decidable for the quantifier-free.

**Natural Numbers and Integers** $\mathcal{T}_N$, $\mathcal{T}_Z$: the semantic theory of natural numbers (with operations 0, succ, $+$, $\ast$) and integers. It is neither axiomatisable nor decidable (Gödel incompleteness theorem).

**Peano Arithmetic** $\mathcal{T}_{PA}$: a first-order approximation of the theory of natural numbers. Its axiomatisation includes an axiom scheme for induction

$$
\begin{align*}
\phi [0/x] & \\
\forall n. \phi [n/x] & \rightarrow \phi [n + 1/x] \\
\forall n. \phi [n/x]
\end{align*}
$$

It is incomplete and undecidable (even for the quantifier-free fragment).

**Linear Arithmetic** $\mathcal{T}_{LA}$: with vocabulary $V = \{ \ldots , -2, -1, 0, 1, 2, \ldots , 2n, -1n, 1n, 2n, \ldots , +, =, < \}$, where $n$ is a unary function that multiplies its argument by a constant. This theory is both complete and decidable, and it is in fact one of the most widely used in the context of program verification.

**Rational Numbers**: the full theory of rational numbers (with addition and multiplication) is undecidable, since the property of being a natural number can be encoded in it. But the theory of linear arithmetic over rational numbers $\mathcal{T}_{QLA}$ is decidable, and actually more efficiently than the corresponding theory of integers.

**Reals** $\mathcal{T}_R$: surprisingly, this theory is decidable even in the presence of multiplication and quantifiers. However, the time complexity of the associated decision procedure may make its application prohibitive.

**Fixed-size bit vectors**: model bit-level operations of machine words, including $2^n$-modular operations (where $n$ is the word size), shift operations, etc. Decision procedures for the theory of fixed-sized bit vectors often rely on appropriate encodings in propositional logic.

**Arrays, Finite Maps, Lists...**
The SMT problem is a variation of the propositional SAT problem for first-order logic, with the interpretation of symbols constrained by (a combination of) specific theories.

More precisely, SMT solvers address the issue of satisfiability of quantifier-free first-order CNF formulas, using as building blocks:

- a propositional SAT-solver,
- and state-of-the-art theory-solvers.

For a first-order CNF $\phi$:

- Let $\text{prop}(-)$ be a map from first-order formulas to propositional formulas that substitutes every atomic formula by a fresh propositional symbol.
- For a valuation $\rho$ of $\text{prop}(\phi)$, the set $\Phi(\rho)$ of first-order literals be defined as follows:
  \[
  \Phi(\rho) = \{ \text{prop}^{-1}(P_i) \mid \rho(P_i) = T \} \cup \{ \neg \text{prop}^{-1}(P_i) \mid \rho(P_i) = F \}
  \]

Given a CNF, the SAT-solver answers either “unsat”, or “sat” with a particular valuation (model).

Given a conjunction of atomic formulas, the theory-solver answers either “$T$-consistent”, or “$T$-inconsistent” with a particular “unsatisfiable kernel” (i.e. a subset of the given set that is already unsatisfiable).

The SMT loop invokes the propositional SAT solver with a propositional formula $A$ that is initialised with $\text{prop}(\psi)$.

If a valuation $\rho$ satisfying $A$ is found, the theory solver is invoked to check if $\Phi(\rho)$ is satisfiable.

If not, it will add to $A$ a clause which will have the effect of excluding $\rho$ when the SAT solver is invoked again in the next iteration.

The algorithm stops whenever the SAT solver returns “unsat”, in which case $\psi$ is unsatisfiable,

or the theory solver returns “sat”, in which case $\psi$ is satisfiable.
Consider the formula

$$g(a) = x \land (f(g(a)) \neq f(c) \lor g(a) = d) \land c \neq d$$

- Send to SAT-solver \{\{1\}, \{-2, 3\}, \{-4\}\}. It answers *satisfiable* with model \{1, -2, -4\}.
- Send model to *Theory-solver*. It answers *T-inconsistent*.
- Send to SAT-solver \{\{1\}, \{-2, 3\}, \{-4\}, \{-1, 2, 4\}\}. It answers *satisfiable* with model \{1, 2, 3, -4\}.
- Send model to *Theory-solver*. It answers *T-inconsistent*.
- Send to SAT-solver \{\{1\}, \{-2, 3\}, \{-4\}, \{-1, 2, 4\}, \{-1, -2, -3, 4\}\}. It answers *unsatisfiable*. 