PROLOG.
Substitutions and Unification

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The role of substitutions

- **Substitution** is an operation allowing to replace some variables occurring in a formula with terms.
- The goal of applying a substitution is to make a certain formula more specific so that it matches another formula. Substitutions allow for unification of formulae (or terms).

Definition

A substitution $\sigma$ is any finite mapping of variables into terms of the form

$$\sigma : V \rightarrow TER.$$  

Notation of substitutions

- Any (finite) substitution $\sigma$ can be presented as

$$\sigma = \{X_1/t_1, X_2/t_2, \ldots, X_n/t_n\},$$

where $t_i$ is a term to be substituted for variable $X_i$, $i = 1, 2, \ldots, n$.
- $\Phi \sigma$ is the formula (or term) resulting from simultaneous replacement of the variables of $\Phi$ with the appropriate terms of $\sigma$. 
Any substitution $\sigma (\sigma : V \rightarrow TER)$ is extended to operate on terms and formulae so that a finite mapping of the form

$$\sigma : TER \cup FOR \rightarrow TER \cup FOR$$

satisfying the following conditions is induced:

- $\sigma(c) = c$ for any $c \in C$;
- $\sigma(X) \in TER$, and $\sigma(X) \neq X$ for a certain finite number of variables only;
- if $f(t_1, t_2, \ldots, t_n) \in TER$, then
  $$\sigma(f(t_1, t_2, \ldots, t_n)) = f(\sigma(t_1), \sigma(t_2), \ldots, \sigma(t_n));$$
- if $p(t_1, t_2, \ldots, t_n) \in ATOM$, then
  $$\sigma(p(t_1, t_2, \ldots, t_n)) = p(\sigma(t_1), \sigma(t_2), \ldots, \sigma(t_n));$$
- $\sigma(\Phi \diamond \Psi) = \sigma(\Phi) \diamond \sigma(\Psi)$ for any two formulae $\Phi, \Psi \in FOR$ and for
  $\diamond \in \{\land, \lor, \Rightarrow, \Leftrightarrow\}$. 
An Instance

Any formula \( \sigma(\Phi) \) resulting from application of substitution \( \sigma \) to the variables of \( \Phi \) will be denoted as

\[ \Phi \sigma \]

and it will be called a substitution instance or simply an instance of \( \Phi \).

A Ground Instance, Term Formula

If no variables occur in \( \Phi \sigma \), it will be called a ground instance (a ground formula or a ground term, respectively).

Example

Let \( \sigma = \{X/a, Y/f(b)\} \), and let \( \Phi = p(X, Y, g(X)) \). Then

\[ \Phi \sigma = p(a, f(b), g(a)) \]

and it is a ground formula.
Since substitutions are mappings, a composition of substitutions is well defined. Having two substitutions, say \( \sigma \) and \( \theta \), the composed substitution \( \sigma \theta \) can be obtained from \( \sigma \) by:

- **simultaneous** application of \( \theta \) to all the terms of \( \sigma \),
- deletion of any pairs of the form \( X/t \) where \( t = X \) (identity substitutions), and
- enclosing all the pairs \( X/t \) of \( \theta \), such that \( \sigma \) does not substitute for (operate on) \( X \).

More formally:

Let \( \sigma = \{X_1/t_1, X_2/t_2, \ldots, X_n/t_n\} \) and let \( \theta = \{Y_1/s_1, Y_2/s_2, \ldots, Y_m/s_m\} \). The composition of the above substitutions is obtained from the set

\[
\{X_1/t_1 \theta, X_2/t_2 \theta, \ldots, X_n/t_n \theta, Y_1/s_1, Y_2/s_2, \ldots, Y_m/s_m\}
\]

by:

- **removing** all the pairs \( X_i/t_i \theta \) where \( X_i = t_i \theta \), and
- **removing** all the pairs \( Y_j/s_j \) where \( Y_j \in \{X_1, X_2, \ldots, X_n\} \).
Consider the following substitutions:

$$\sigma = \{X/g(U), Y/f(Z), V/W, Z/c\}$$

and

$$\theta = \{Z/f(U), W/V, U/b\}.$$

The composition of them is defined as: ???
Consider the following substitutions:

$$\sigma = \{X/g(U), Y/f(Z), V/W, Z/c\}$$

and

$$\theta = \{Z/f(U), W/V, U/b\}.$$ 

The composition of them is defined as:

$$\sigma\theta = \{X/g(b), Y/f(f(U)), Z/c, W/V, U/b\}.$$
Renaming and Inverse Substitutions

**A Renaming Substitution**

Substitution $\lambda$ is a renaming substitution iff it is off the form

$$\theta = \{X_1/Y_1, X_2/Y_2, \ldots, X_n/Y_n\}$$

(1)

Moreover, it is a one-to-one mapping if $Y_i \neq Y_j$ for $i \neq j, i, j \in \{1, 2, \ldots, n\}$.

**An Inverse Substitution**

Assume $\lambda$ is a renaming, one-to-one substitution. The inverse substitution for it is given by

$$\lambda^{-1} = \{Y_1/X_1, Y_2/X_2, \ldots, Y_n/X_n, \}.$$  

**Composition of inverse substitutions**

The composition of a renaming substitution and the inverse one leads to an empty substitution, traditionally denoted with $\epsilon$; we have

$$\lambda \lambda^{-1} = \epsilon.$$
An Instance

Let $E$ denote an expression (formula or term), $\epsilon$ denote an empty substitution, and let $\lambda$ be a one-to-one renaming substitution; $\sigma$ and $\theta$ denote any substitutions. The following properties are satisfied for any substitutions:

- $E(\sigma \theta) = (E \sigma) \theta$,
- $\sigma(\theta \gamma) = (\sigma \theta) \gamma$ (associativity),
- $E \epsilon = E$,
- $\epsilon \sigma = \sigma \epsilon = \sigma$.

Note that, in general, the composition of substitutions is not commutative.
Substitutions are applied to *unify* terms and formulae. Unification is a process of determining and applying a certain substitution to a set of expressions (terms or formulae) in order to make them identical. We have the following definition of unification.

**Definition**

Let \( E_1, E_2, \ldots, E_n \in \text{TER} \cup \text{FOR} \) are certain expressions. We shall say that expressions \( E_1, E_2, \ldots, E_n \) are *unifiable* if and only if there exists a substitution \( \sigma \), such that

\[
\{E_1, E_2, \ldots, E_n\} \sigma = \{E_1\sigma, E_2\sigma, \ldots, E_n\sigma\}
\]

is a single-element set.

Substitution \( \sigma \) satisfying the above condition is called a *unifier* (or a *unifying substitution*) for expressions \( E_1, E_2, \ldots, E_n \).

Note that if there exists a unifying substitution for some two or more expressions (terms or formulae), then there usually exists more than one such substitution (or even infinitely many unifiers).
The Most General Unifier (mgu)

It is useful to define the so-called *most general unifier* (mgu, for short), which, roughly speaking, substitutes terms for variables only if it is necessary, leaving as much place for possible further substitutions, as possible.

**Definition**

A substitution $\sigma$ is a *most general unifier* for a certain set of expressions if and only if, for any other unifier $\theta$ of this set of expressions, there exists a substitution $\lambda$, such that $\theta = \sigma \lambda$.

The meaning of the above definition is obvious. Substitution $\theta$ is not a most general unifier, since it is a composition of some simpler substitution $\sigma$ with an auxiliary substitution $\lambda$.

In general, for arbitrary expressions there may exist an infinite number of unifying substitutions. However, it can be proved that any two most general unifiers can differ only with respect to variable names. This is stated with the following theorem.

**A Theorem**

Let $\theta_1$ and $\theta_2$ be two most general unifiers for a certain set of expressions. Then, there exists a one-to-one renaming substitution $\lambda$ such that $\theta_1 = \theta_2 \lambda$ and $\theta_2 = \theta_1 \lambda^{-1}$.
As an example consider atomic formulae $p(X,f(Y))$ and $p(Z,f(Z))$. The following substitutions are all most general unifiers:

- $\theta = \{X/U, Y/U, Z/U\}$,
- $\theta_1 = \{Z/X, Y/X\}$,
- $\theta_2 = \{X/Y, Z/Y\}$,
- $\theta_3 = \{X/Z, Y/Z\}$.

All of the above unifiers are equivalent — each of them can be obtained from another one by applying a renaming substitution. For example, $\theta = \theta_1 \lambda$ for $\lambda = \{X/U\}$; on the other hand obviously $\theta_1 = \theta \lambda^{-1}$. 
It can be proved that if the analyzed expressions are terms or formulae, then there exists an algorithm for efficient generating the most general unifier, provided that there exists one; in the other case the algorithm terminates after finite number of steps. Hence, the unification problem is decidable.

The basic idea of the unification algorithm can be explained as a subsequent search through the structure of the expressions to be unified for inconsistent relative components and replacing one of them, hopefully being a variable, with the other.

In order to find inconsistent components it is useful to define the so-called disagreement set.

Let \( W \subseteq TER \cup FOR \) be a set of expressions to be unified. A \textit{disagreement set} \( D(W) \) for a nonempty set \( W \) is the set of terms obtained through parallel search of all the expressions of \( W \) (from left to right), which are different with respect to the first symbol. Hence, the set \( D(W) \) specifies all the inconsistent relative elements met first during the search.
1. Set $i = 0$, $W_i = W$, $\theta_i = \epsilon$.

2. If $W_i$ is a singleton, then stop; $\theta_i$ is the most general unifier for $W$.

3. Find $D(W_i)$.

4. If there are a variable $X \in D(W_i)$ and a term $t \in D(W_i)$, such that $X$ does not occur in $t$, then proceed; otherwise stop — $W$ is not unifiable.

5. Set $\theta_{i+1} = \theta\{X/t\}$, $W_{i+1} = W_i\{X/t\}$.

6. Set $i = i + 1$ and go to 2.
Consider two atomic formulae \( p(X,f(X,Y), g(f(Y,X))) \) and \( p(c,Z, g(Z)) \). The following steps illustrate the application of the unification algorithm to these atomic formulae.

1. \( i = 0, W_0 = \{ p(X,f(X,Y), g(f(Y,X))), p(c,Z, g(Z)) \}, \theta_0 = \{ \} \).
2. \( D(W_0) = \{ X, c \} \).
3. \( \theta_1 = \{ X/c \}, W_1 = \{ p(c,f(c,Y), g(f(Y,c))), p(c,Z, g(Z)) \} \).
4. \( D(W_1) = \{ f(c,Y), Z \} \).
5. \( \theta_2 = \{ X/c \}\{ Z/f(c,Y) \} = \{ X/c, Z/f(c,Y) \}, W_2 = \{ p(c,f(c,Y), g(f(Y,c))), p(c,f(c,Y), g(f(c,Y))) \} \).
6. \( D(W_2) = \{ Y, c \} \).
7. \( \theta_3 = \{ X/c, Z/f(c,Y) \}\{ Y/c \} = \{ X/c, Z/f(c,c), Y/c \}, W_3 = \{ p(c,f(c,c), g(f(c,c))), p(c,f(c,c), g(f(c,c))) \} \).
8. Stop; the most general unifier is \( \theta_3 = \{ X/c, Z/f(c,c), Y/c \} \).
Properties of the Unification Algorithm

Theorem

1. If $W$ is a finite set of unifiable expressions, then
   - the Unification Algorithm always terminates at step 2 and
   - it produces the most general unifier for $W$.

2. Moreover, if the expressions of $W$ are not unifiable, then the algorithm terminates at step 4.
From: R. Bartak:

Unification Algorithm defined in Prolog

```
unify(A,B):-
    atomic(A), atomic(B), A=B.
unify(A,B):-
    var(A), A=B.  % without occurs check
unify(A,B):-
    nonvar(A), var(B), A=B.  % without occurs check
unify(A,B):-
    compound(A), compound(B),
    A=..[F|ArgsA], B=..[F|ArgsB],
    unify_args(ArgsA,ArgsB).
unify_args([A|TA],[B|TB]):-
    unify(A,B),
    unify_args(TA,TB).
unify_args([],[]).
```

Question
Are $X$ and $f(X)$ unifiable?

Example
What is/should be the result of:
?- $X=f(X)$.
?- $X=a$, $X=f(X)$.
?- $X=f(X)$, write($X$).