gw 7/4/10

Prelude to 'Notes on Compression' ①

A broader category (cf. Russ's 1st Barbados talk)

Assume:

a set of agent names Nme;
a set of site identifiers $SiteId$.
~~a set of property identifiers PropId~~.

A *signature* Σ comprises a function

$$\Sigma_0 : Nme \longrightarrow \mathcal{P}_{fin}(SiteId)$$

together with a set of site-properties

$$\Sigma_1 .$$

[Site-properties identify properties such as 'phosphorylated', 'unphosphorylated', etc. They do not include 'is externally linked', which will require a separate treatment.]

A *Σ-graph* comprises

• a set of *agents* Ag with name function $nme : Ag \longrightarrow Nme$;

• a set of *sites* $Sts \subseteq \{(A,i) \mid i \in \Sigma_0\, nme(A)\}$

with a function $ag : Sts \to Ag$ s.t. $ag(A,i) = A$;

- a set of <u>links</u> $Lnk \subseteq Sts \times Sts$ forming a symmetric relation, with source and target maps src and tar giving the lhs and rhs of a link;

- a set $ExtLnk \subseteq Sts$ specifying those sites with an 'external link'; 

- a subset $P_k \subseteq Sts$ for each $k \in \Sigma_1$.

Two special cases:

A (Σ-) <u>contact graph</u> is a Σ-graph where the set of agents equals Nme, and sites are

$$\{(n,i) \mid n \in Nme \ \& \ i \in \Sigma_0(n)\}.$$

A (Σ-) <u>site graph</u> is a Σ-graph in which the link relation Lnk is irreflexive, its source and target maps are injective and

$$((A,i),(B,j)) \in Lnk \Rightarrow (A,i) \notin ExtLnk.$$

A homomorphism of Σ-graphs

$$h : (Ag, Sts, Lnk, ExtLnk, \{P_k\}_{k \in \Sigma_1}) \longrightarrow$$

$$(Ag', Sts', Lnk', ExtLnk', \{P'_k\}_{k \in \Sigma_1})$$

is a (total) function $h : Ag \to Ag'$ s.t.

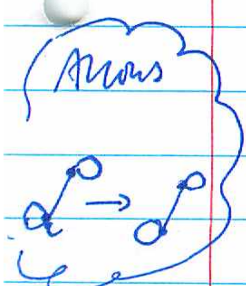
$$(A,i) \in Sts \Rightarrow (h(A), i) \in Sts' ;$$

$$((A,i),(B,j)) \in Lnk \Rightarrow ((h(A),i),(h(B),j)) \in Lnk' ;$$

$$(A,i) \in ExtLnk \Rightarrow (h(A),i) \in ExtLnk' \text{ or } \exists (B,j).\ ((h(A),i),(B,j)) \in Lnk .$$

and

$$h P_k \subseteq P'_k \quad \text{for all } k \in \Sigma_1 .$$



Contact graphs provide type information: that a site graph U has type a contact graph C is represented by a homomorphism

$$t : U \longrightarrow C.$$

Given a homomorphism

$$h : C \longrightarrow C'$$

between contact graphs, we obtain

$$h \circ t : U \longrightarrow C'$$

— a site graph of type C becomes a site graph of type C'. Conversely, we can pull back a site graph of type C' to a site graph of type C:

$$\begin{tikzcd}
U \arrow[r, dashed, "h'"] \arrow[d, dashed, "t"'] \arrow[dr, phantom, very near start, "\lrcorner"] & U' \arrow[d, "t'"] \\
C \arrow[r, "h"'] & C'
\end{tikzcd}$$

Site graphs of type C form a ('comma') category $\tilde{C}$ with maps, homomorphisms l s.t.

$$\begin{tikzcd} U_1 \arrow[rr, dashed, "l"] \arrow[dr, "t_1"'] & \arrow[d, phantom, "="] & U_2 \arrow[dl, "t_2"] \\ & C & \end{tikzcd}$$

The two ways of moving between types $h_*: \tilde{C} \longrightarrow \tilde{C}'$, got by composition with h, and $h^*: \tilde{C}' \longrightarrow \tilde{C}$, ~~from~~ got by pullback along h, extend to functors which are part of an adjunction

$$\begin{tikzcd} \tilde{C} \arrow[r, bend right, "h_*"'] \arrow[r, phantom, "\top"] & \tilde{C}' \arrow[l, bend right, "h^*"'] \end{tikzcd}$$

with h_* left adjoint to h^*.

There are some things to check here. Firstly, pullbacks of homomorphisms on Σ-graphs exist in general. Given homomorphisms of Σ-graphs

$$\begin{tikzcd} & U' \arrow[d, "t"] \\ C \arrow[r, "h"'] & C' \end{tikzcd},$$

then pullback

$$\begin{tikzcd} U \arrow[r, "h'"] \arrow[d, "t'"'] \arrow[dr, phantom, "\lrcorner", very near start] & U' \arrow[d, "t"] \\ C \arrow[r, "h"'] & C' \end{tikzcd}$$

is given explicitly as follows. The agents of U are pairs (c, u') of agents of C and U' s.t. $h(c) = t(u')$. The ~~maps~~ functions t' and h' are given by projections. The extra structure on U, its sites, links and properties are inherited when <u>both</u> C and U' have the structure. E.g. agent (c, u') has site i when <u>both</u> agent c of C ~~has~~ and agent u' of U' have site i, sites are linked in U when both projections are linked, etc.

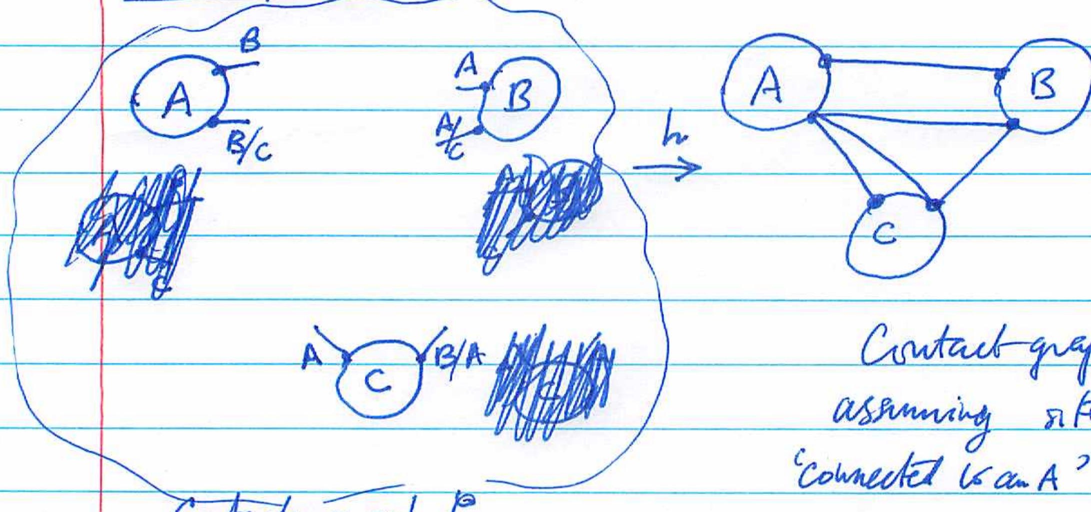
Now, in the special case where C, C' are contact graphs and U' is a site graph, h is mono so h' is too (pbs preserve monos) and all the site-graph structure of U is inherited from U'. ~~For this reason U' is also being a site graph entails U is a site graph too~~

To establish the adjunction $h_* \dashv h^*$ we need a natural bijection between maps $h_*(t_1) \xrightarrow{f} t_2$ in $\tilde{C}'$ and $t_1 \xrightarrow{g} h^*(t_2)$ in $\tilde{C}$. The bijection is summarised in the diagram

$$\begin{tikzcd}
U_1 \arrow[dr, dashed, "g"] \arrow[drr, dashed, bend left, "f"] \arrow[ddr, bend right, "t_1"'] & & \\
& U_2' \arrow[r, "h'"] \arrow[d, "t_2'"] \arrow[dr, phantom, very near start, "\lrcorner"] & U_2 \arrow[d, "t_2"] \\
& C \arrow[r, "h"'] & C'
\end{tikzcd}$$

where $h_*(t_1) = h \circ t_1$ and $h^*(t_2) = t_2'$: given f we obtain g by the universal property of pullback; given g we obtain f by composition with h'. That these procedures are mutually inverse follows from ~~the~~ universality. ~~property of pb.~~

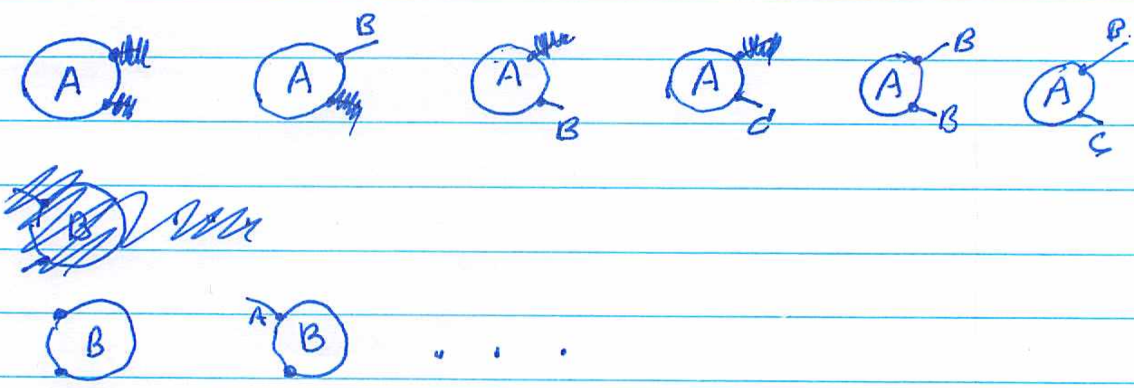
Example



Contact graph $\mathcal{C}'$.
assuming site properties
'connected to an A' etc.

Contact graph $\mathcal{C}$
with site properties 'connected
to an A', '.. to a B', ...

$h^*(T' \xrightarrow{t'} \mathcal{C}')$ would in effect break T' into a multiset of 'fragments': (cf. Jerome's talk)



Such adjunctions could be important in supporting abstract-interpretation techniques.

Partial maps of Σ-graphs

A Σ_0-subgraph of a Σ-graph $(Ag, Sts, Lnk, ExtLnk, \{P_k\}_{k\in\Sigma_0})$ is a Σ-graph $(Ag', Sts', Lnk', ExtLnk', \{\emptyset\}_{k\in\Sigma_0})$ where $Ag' \subseteq Ag$, $Sts' \subseteq Sts$, $Lnk' \subseteq Lnk$ and $ExtLnk' \subseteq ExtLnk$. Σ_0-subgraphs are used to pick out the 'domain of definition' of partial maps, those agents, sites, links and external links on which the map is defined.

A partial map between Σ-graphs comprises

$$\begin{tikzcd} & D \arrow[dl, hook'] \arrow[dr, "h"] & \\ T & & U \end{tikzcd}$$

where D is a Σ_0-subgraph of T and h is a homomorphism. We shall identify homomorphisms $h : T \to U$ with partial maps

$$\begin{tikzcd} & T_\emptyset \arrow[dl, hook'] \arrow[dr, "h"] & \\ T & & U \end{tikzcd}$$

in which $T_\emptyset$ is the Σ_0-subgraph obtained from

T by setting all its site properties to $\emptyset$.

Let $h : T \to U$ be a homomorphism and U' a Σ_0-subgraph of U. Define its inverse image $h^{-1}U'$ to be the Σ_0-subgraph of T obtained as the componentwise inverse image of U' under h, viz.

- its agents are all $A \in Ag_T$ s.t. $h(A) \in Ag_{U'}$;
- sites are all $(A,i) \in Sts_T$ s.t. $(h(A),i) \in Sts_{U'}$;
- links are all $((A,i),(B,j)) \in Lnk_T$ s.t. $((h(A),i),(h(B),j)) \in Lnk_{U'}$;
- external links are all $(A,i) \in ExtLnk_T$ s.t. either $(h(A),i) \in ExtLnk_{U'}$ or $\exists (B,j).\ ((h(A),i),(B,j)) \in Lnk_{U'}$.

[Note the extra wrinkle in the external-links case.]

We obtain:

$$\begin{tikzcd} T \arrow[r, "h"] & U \\ h^{-1}U' \arrow[u, hook] \arrow[r, "h'"'] \arrow[ur, phantom, "="] & U' \arrow[u, hook] \end{tikzcd}$$

in which h' is a homomorphism, got by restricting h.

Assume partial maps of Σ-graphs

$$\begin{tikzcd} & D \arrow[dl, hook'] \arrow[dr, "h"] & \\ T & & U \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} & D' \arrow[dl, hook'] \arrow[dr, "k"] & \\ U & & V \end{tikzcd} .$$

Their composition is obtained as:

$$\begin{tikzcd} & & h^{-1}D' \arrow[dl, hook'] \arrow[dr, "h'"] & & \\ & D \arrow[dl, hook'] \arrow[dr, "h"] & & D' \arrow[dl, hook'] \arrow[dr, "h'"] & \\ T & & U & & V \end{tikzcd}$$

Note that, as defined, a partial map of Σ-graphs cannot send an internal link $\circ\!-\!\circ$ to an external link $\circ\!-$, though the converse is possible both for partial maps and homomorphisms.

An alternative view of partial maps of site-graphs.

A partial map of site graphs

$$f : T \longrightarrow U$$

corresponds to componentwise partial maps f, f_{sts}, f_{lnk}, f_{ext}, f_{extint}

$$
\begin{tikzcd}
Nme \arrow[d, equal] & Ag_T \arrow[l, "name_T"'] \arrow[d, "f"] \arrow[dl, phantom, "\supseteq"] & Sts_T \arrow[l, "ag_T"'] \arrow[d, "f_{sts}"] \arrow[dl, phantom, "\supseteq"] & Lnk_T \arrow[l, bend right, "src_T"'] \arrow[l, bend left, "tar_T"] \arrow[d, "f_{lnk}"] \arrow[dl, phantom, "\supseteq"] \\
Nme & Ag_U \arrow[l, "name_U"] & Sts_U \arrow[l, "ag_U"] & Lnk_U \arrow[l, bend right, "src_U"'] \arrow[l, bend left, "tar_U"]
\end{tikzcd}
$$

$$
\begin{tikzcd}
Sts_T \arrow[d, "f_{sts}"] & & ExtLnk_T \arrow[ll, hook'] \arrow[rr, hook] \arrow[dl, "f_{ext}"'] \arrow[dr, "f_{extint}"] & & Sts_T \arrow[d, "f_{sts}"] \\
Sts_U \arrow[ur, phantom, "\supseteq"] & ExtLnk_U \arrow[l, hook'] & & Lnk_U \arrow[r, "src_U"'] \arrow[ur, phantom, "\subseteq"] & Sts_U
\end{tikzcd}
$$

where f_{ext}, f_{extint} have disjoint domains of definition, satisfying the partial commutativity conditions shown. An external link of T ~~or~~ may go to an external link of U or to an internal link of U — for a site graph U at most ~~only~~ one of these possibilities can occur.

Composition of partial graphs, $f : T \to U$ and $g : U \to V$ corresponds to componentwise composition in the above reformulation, though with the following qualification for maps of external links:

$$\begin{tikzcd}
 & \mathrm{ExtLnk}_T \arrow[dl, "f_{ext}"'] \arrow[dr, "f_{extint}"] & \\
\mathrm{ExtLnk}_U \arrow[d, "g_{ext}"'] \arrow[drr, "g_{extint}"] & & \mathrm{Lnk}_U \arrow[d, "g_{lnk}"] \\
\mathrm{ExtLnk}_V & & \mathrm{Lnk}_V
\end{tikzcd}$$

$$(g \circ f)_{ext} = g_{ext} \circ f_{ext}$$

$$(g \circ f)_{extint} = g_{extint} \circ f_{ext} \cup g_{lnk} \circ f_{extint}$$

Special maps

Embeddings A homomorphism of Σ-graphs $f : S \to T$ is an *embedding* if f is injective

$$((f(A),i),(f(B),j)) \in \mathrm{Lnk}_T \Rightarrow ((A,i),(B,j)) \in \mathrm{Lnk}_S,$$
$$((f(A),i),(B,j)) \in \mathrm{Lnk}_T \;\&\; B \notin \mathrm{rge}\, f \Rightarrow (A,i) \in \mathrm{ExtLnk}_S, \text{ and}$$
$$(f(A),i) \in \mathrm{ExtLnk}_T \Rightarrow (A,i) \in \mathrm{ExtLnk}_S.$$

As for homomorphisms in general, we can regard embeddings as (special) partial maps.

Action maps A partial map of Σ-graphs $f : S \to S'$ is an *action* map if

f is partial injective (i.e. $f(A) = f(B)$, both defined, implies $A = B$), and ~~provided if f(A) is defined~~ if $f(A) = A'$,

$$(A,i) \in \mathrm{Sts}_S \Leftrightarrow (A',i) \in \mathrm{Sts}_{S'}, \text{ and}$$

$$(A,i) \in \mathrm{ExtLnk}_S \Leftrightarrow (A',i) \in \mathrm{ExtLnk}_{S'};$$

A created or deleted agent has all pristine sites

if $f(A)$ undefd, $(A,i) \in \mathrm{Sts}_S$ for all $i \in \Sigma\mathrm{nme}\,A$;

if $A' \notin \mathrm{rge}\, f$, $(A',i) \in \mathrm{Sts}_{S'}$ for all $i \in \Sigma\mathrm{nme}(A')$.

An action map $f : S \to S'$ is a special partial map

$$\begin{tikzcd} & D \arrow[dl] \arrow[dr, "h"] & \\ S & & S' \end{tikzcd}$$

where D is a Σ_0-subgraph of S and h is an injective function forming a homomorphism from D to S. Because f is an action map $h\,ExtLinks_D \subseteq ExtLinks_{S'}$.

Consequently, we can rename D to obtain

$$\begin{tikzcd} & \bar{D} \arrow[dl, "\bar{h}"'] \arrow[dr, hook] & \\ S & & S' \end{tikzcd},$$

a reverse $f^{op} : S' \to S$ of the action map $f : S \to S'$.

__Proposition__ If $f : S \to S'$ is an action map then so is its ~~converse~~ reverse $f^{op} : S' \to S$.

<u>Proposition</u> A pair of maps

$$\begin{array}{ccc} S & \xrightarrow{\alpha} & S' \\ \varphi \big\downarrow & & \\ T & & \end{array}$$

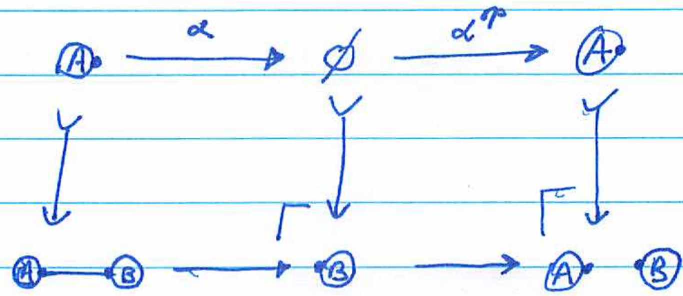
where φ is an embedding, α is an action map and S, S', T are site graphs has a pushout in the category of Σ-graphs with partial maps. The pushout takes the form

$$\begin{array}{ccc} S & \xrightarrow{\alpha} & S' \\ \varphi \big\downarrow & & \big\downarrow \varphi' \\ T & \xrightarrow[\alpha']{} & T' \end{array}$$

where φ' is an embedding and α' is an action map. If T is a solution, i.e. a complete site graph, then so is T'.

[This and the surrounding generalisations, eg. to all Σ-graphs needs to be checked carefully.]

Although action maps are reversible, pushout w.r.t. to an action map followed by pushout w.r.t. its reverse need not return the ~~set~~ initial solution (up to iso). An example of Vincent:



Link structure is lost in the deletion followed by creation of A. The example also shows, by considering the rhs pushout, why creation rules have to create agents with all their sites — otherwise solutions ~~to~~ would not necessarily go to solutions under actions. [To maintain reversibility of action maps we must then only allow delete actions when all sites are present in the deleted agent.]

I think the following is true. Provided α doesn't delete agents:

$$\begin{tikzcd} S \arrow[r, "\alpha"] \arrow[d, tail] & S' \arrow[r, "\alpha^{op}"] \arrow[d, tail] & S \arrow[d, tail] \\ T \arrow[r, "\alpha'"'] & T' \arrow[r, "\alpha^{op\prime}"'] & T'' \end{tikzcd} \quad \Rightarrow T \cong T''$$

(the isomorphism induced by the function on agents in $\alpha^{op\prime} \circ \alpha'$ (this need not itself be an iso, eg. links might be dropped).

<u>Remark [Vincent]</u> The 'standard' graph rewrite technique of 'double pushout' does not work ~~for~~ on site graphs: Action map

$$A\bullet \longrightarrow B$$

deleting $A\bullet$ and creating B ~~work~~ stands for a span

$$\begin{tikzcd} & \emptyset \arrow[dl] \arrow[dr] & \\ A\bullet & & B \end{tikzcd}$$

The kappa rewrite

$$\begin{tikzcd} A\bullet \arrow[r] \arrow[d, tail] & B \arrow[d, tail] \\ A\bullet\!\!-\!\!\bullet C \arrow[r] & B \quad \bullet C \end{tikzcd}$$

cannot be carried out as a double pushout:

$$\begin{tikzcd} A\bullet \arrow[d, tail] & \emptyset \arrow[l] \arrow[r] \arrow[d] & B \arrow[d, dotted] \\ A\bullet\!\!-\!\!\bullet C & ? \arrow[l] \arrow[r, dotted] & {} \end{tikzcd}$$

as there's no fill-in for '?' making the lhs a pushout (in the category of Σ-graphs with homomorphisms).