Process Algebras & Network Motifs

section 3

Process algebras and network motifs 3

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Michaelis-menten revisited

$$E + S \leftrightarrow^{k1}_{k\text{-}1} ES \rightarrow^{k2} E + P$$

- Says nothing about **internal** structure of E, S, P, ES
- Priami/Regev/Shapiro encoding gives detailed account of the internal structure of these agents
- Does not give detailed account of scope of the encoding… we want to encode the **reaction**… but according to certain principles

$$[E + S \leftrightarrow^{k1}_{k\text{-}1} ES \rightarrow^{k2} E + P]_\pi$$

- $[\, - \rightarrow_{\mathrm{chem}} - \,]_\pi = - \rightarrow_\pi^* -$
- $[\, - +_{\mathrm{chem}} - \,]_\pi = - \mid -$

Michaelis-menten revisited

$$E + S \leftrightarrow {}^{k1}{}_{k\text{-}1}\, ES \rightarrow {}^{k2}\, E + P$$

From these we deduce

- $[E + S]_\pi = [E]_\pi \mid [S]_\pi \rightarrow_\pi^* [ES]_\pi$
- $[ES]_\pi \rightarrow_\pi^* ([E]_\pi \mid [S]_\pi) + ([E]_\pi \mid [P]_\pi)$

From these we deduce

- $\exists x_0 . ([E]_\pi \approx (\upsilon\, e)(x_0[e].[E]_\pi' + X_E))\ \&\ ([S]_\pi \approx x_0(y).[S]_\pi' + X_S)$
- $[ES]_\pi \approx (\upsilon\, e)([E]_\pi' \mid [S]_\pi'\{e/y\})$

Therefore

- $(\upsilon\, e)([E]_\pi' \mid [S]_\pi'\{e/y\}) \rightarrow_\pi^* ([E]_\pi \mid [S]_\pi) + ([E]_\pi \mid [P]_\pi)$

Michaelis-menten revisited

$$E + S \leftrightarrow^{k1}_{k-1} ES \rightarrow^{k2} E + P$$

Since E is and enzyme, $[E]_\pi$ is the future of $[E]_\pi'$,
and $[S]_\pi$ and $[P]_\pi$ are the futures of $[S]_\pi'\{e/y\}$

- $(\upsilon\ e)([E]_\pi' \mid [S]_\pi'\{e/y\}) \rightarrow_\pi^* ([E]_\pi \mid [S]_\pi) + ([E]_\pi \mid [P]_\pi)$

Implies

- $\exists x_1 x_2.([E]_\pi' \approx x_1(y).[E]_\pi + x_2(y).[E]_\pi + X_{E'}) \& ([S]_\pi' \approx x_1[e].[S]_\pi + x_2[e].[P]_\pi + X_{S'})$

Setting X's to 0 and minimizing the number of $\rightarrow_\pi$ steps
we arrive at

- $[E]_\pi = (\upsilon\ e)(x_0[e].(x_1(y).[E]_\pi + x_2(y).[E]_\pi))$
- $[S]_\pi = x_0(y).(x_1[e].[S]_\pi + x_2[e].[P]_\pi)$

Michaelis-menten revisited

1. The Priami/Regev/Shapiro encoding is in some sense the smallest process satisfying the logical constraints of the chemical equation
2. Our more careful derivation of that process exhibits some of the other processes that also exhibit that behavior
   - Michaelis-Menten is a scheme -- a logical property -- that lots of networks might enjoy
3. Is there an account of this logical entity in the process algebra setting? Yes!
   - We propose a translation, $[-]_{\varphi}$, of the **logical content** of reaction into spatial logic

Michaelis-menten revisited

$$[E + S \leftrightarrow^{k1}_{k-1} ES \rightarrow^{k2} E + P]_{\varphi}$$

- $[- \rightarrow_{\text{chem}} -]_{\varphi} = - \Rightarrow \Diamond -$
- $[- +_{\text{chem}} -]_{\varphi} = - \mid -$
- $[A]_{\varphi}$ denotes the *characteristic formula* of the process representing A
- $[A]_{\pi} \setminus [A]_{\varphi}$

Thus, in our example

- $[E\,]_{\varphi} | [S]_{\varphi} \Rightarrow \mathsf{N}[ES]_{\varphi}$
- $[ES]_{\varphi} \Rightarrow \mathsf{N}([E\,]_{\varphi} | [S]_{\varphi}) \mathbin{\&} \mathsf{N}\,([E\,]_{\varphi} | [P]_{\varphi}) \mathbin{\&} 1$

from which we can conclude

Michaelis-menten revisited

$$[E + S \leftrightarrow^{k1}_{k-1} ES \rightarrow^{k2} E + P]_\varphi$$

If we assume that the **reason** $[ES]_\varphi \Rightarrow 1$ is

$[ES]_\varphi \Rightarrow \Diamond \mathsf{H}e.([E]_\varphi{}'(e) \mid [S]_\varphi{}'(e))$ then

- $\exists x_1 x_2. ([E]_\varphi{}'(e) \Rightarrow \Diamond\langle x_1(y)\rangle[E]_\varphi \& \Diamond\langle x_2(y)\rangle[E]_\varphi)$
  $\& ([S]_\varphi{}'(e) \Rightarrow \Diamond\langle x_1(y)\rangle[S]_\varphi \& \Diamond\langle x_2(y)\rangle[P]_\varphi)$

Taking

- $[E]_\varphi = \mu X. (\Diamond \mathsf{H}e.\langle -x_0[e]\rangle\Diamond\langle x_1(y)\rangle X \& \Diamond\langle x_2(y)\rangle X)$
- $[S]_\varphi = \mu X. (\Diamond\langle x_0(y)\rangle\Diamond\langle x_1[y]\rangle X \& \Diamond\langle x_2[y]\rangle[P]_\varphi)$
- $[ES]_\varphi = \mathsf{H}e.([E]_\varphi \mid [S]_\varphi)$

Guarantees our requirements

But denotes the **set** of networks acting as Michaelis-Menten