Models and Languages for Computational Systems Biology

Lecture 2: Petri Nets

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School of Informatics
The University of Edinburgh

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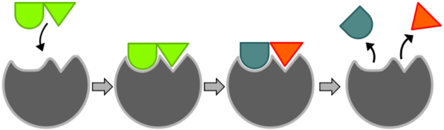
Semester 2 Week 1

Outline

Example: Enzyme Catalysis



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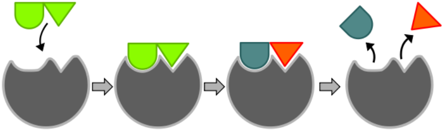

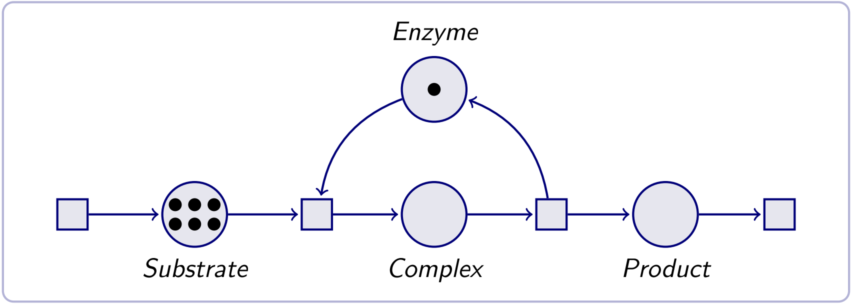

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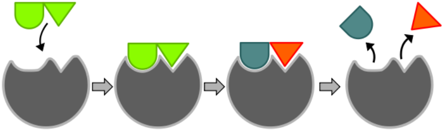

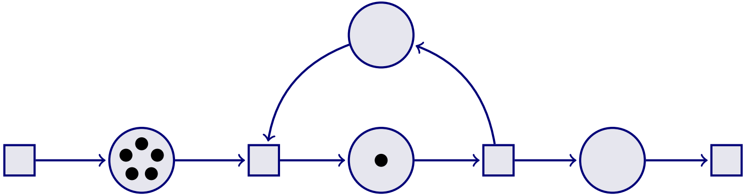

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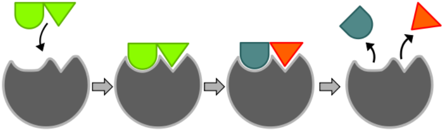

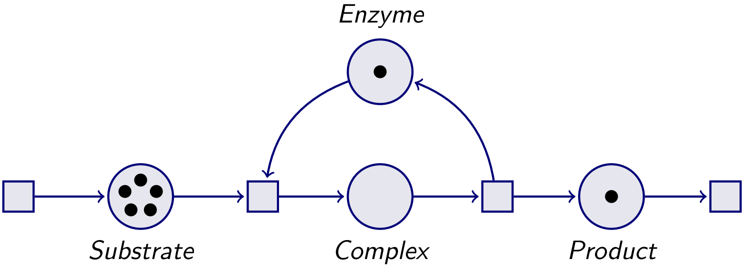

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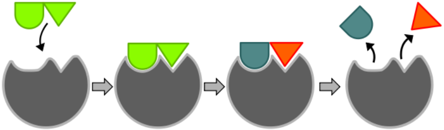

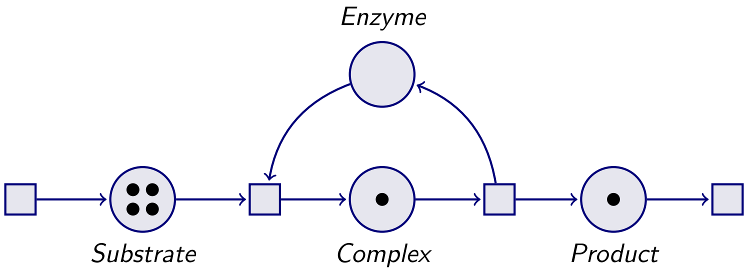

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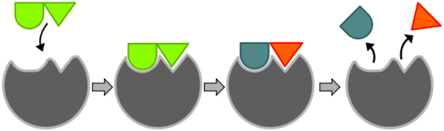

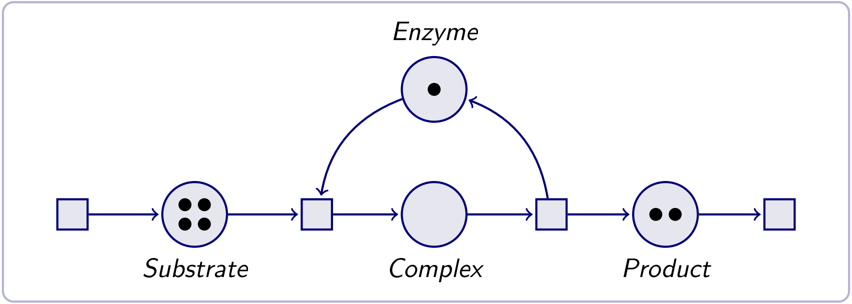

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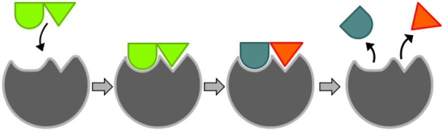

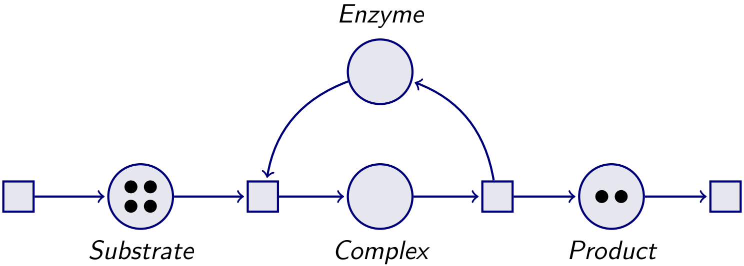

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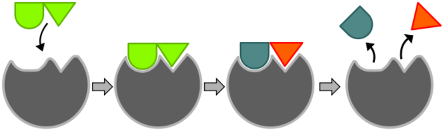

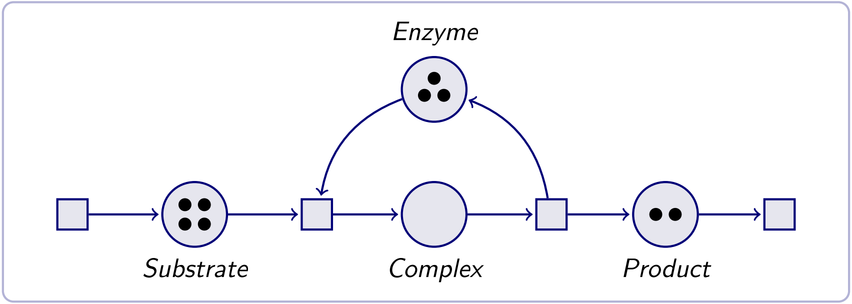

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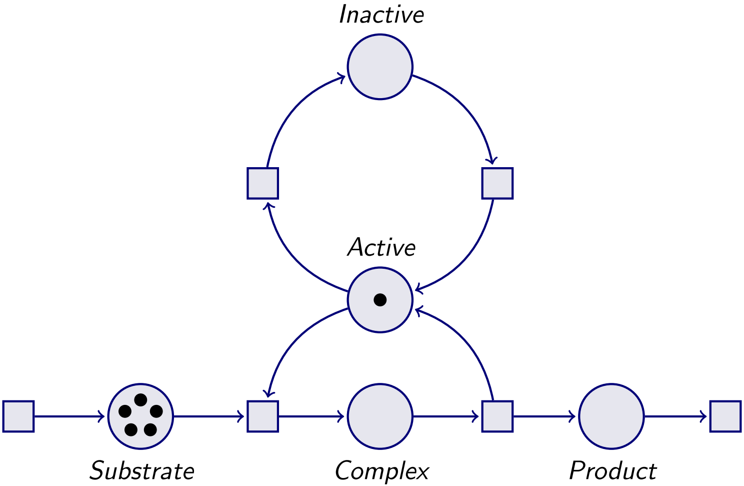

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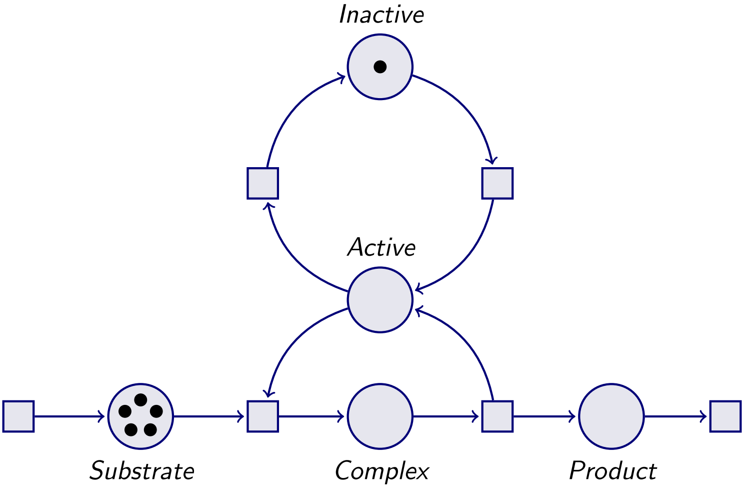

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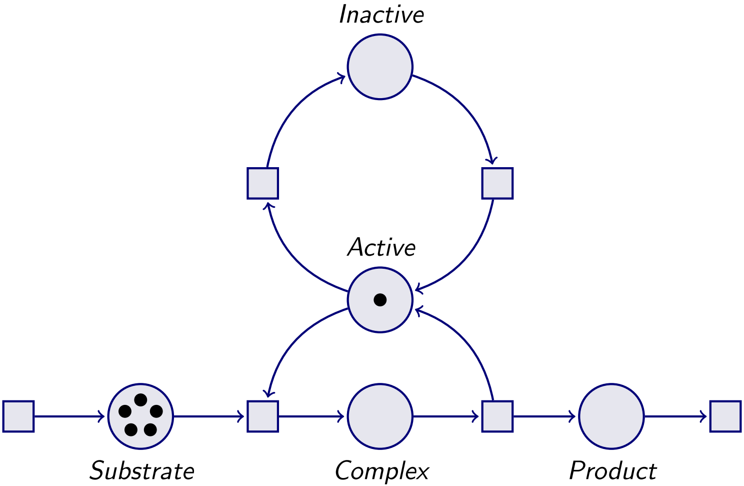

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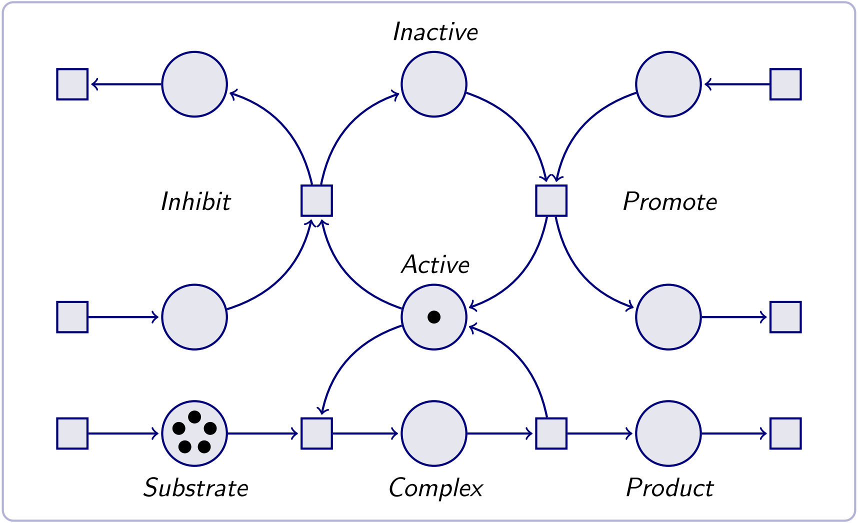

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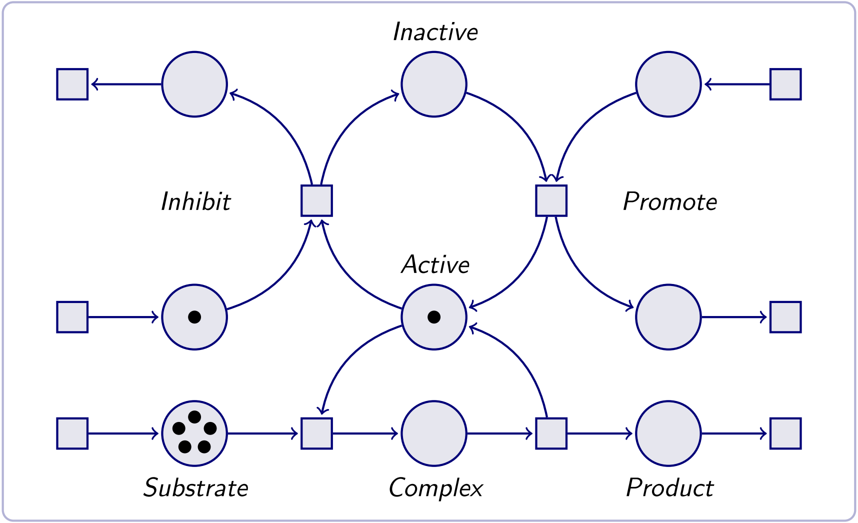

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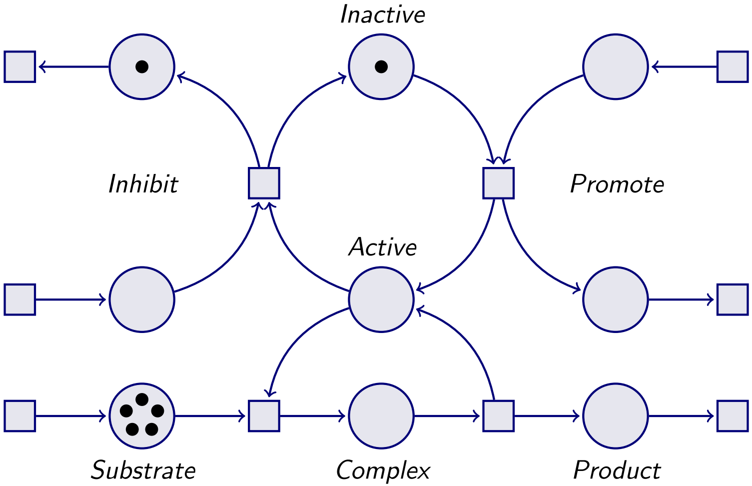

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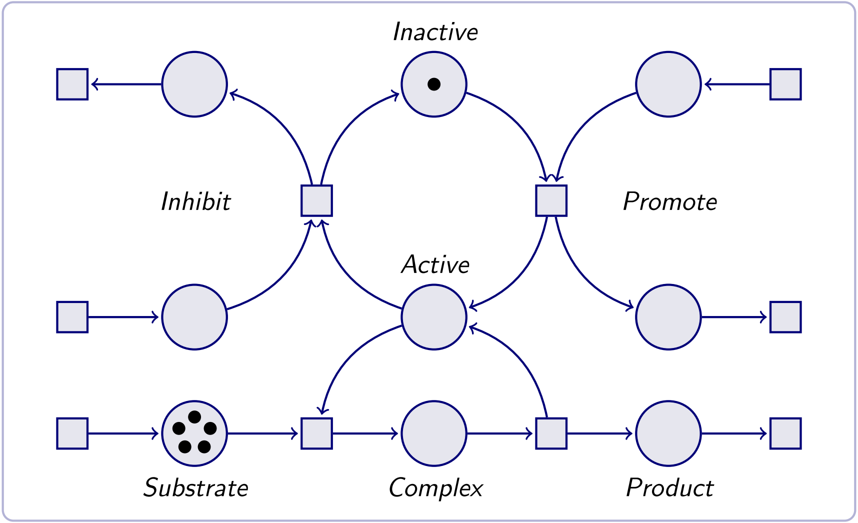

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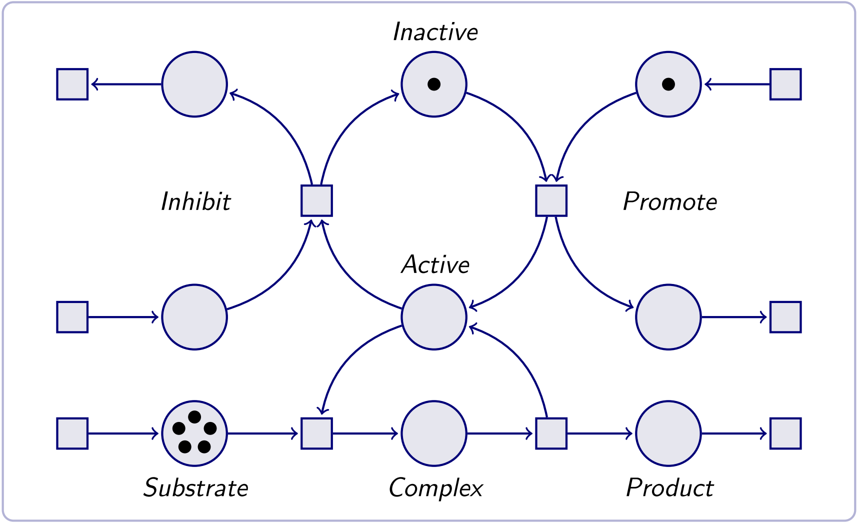

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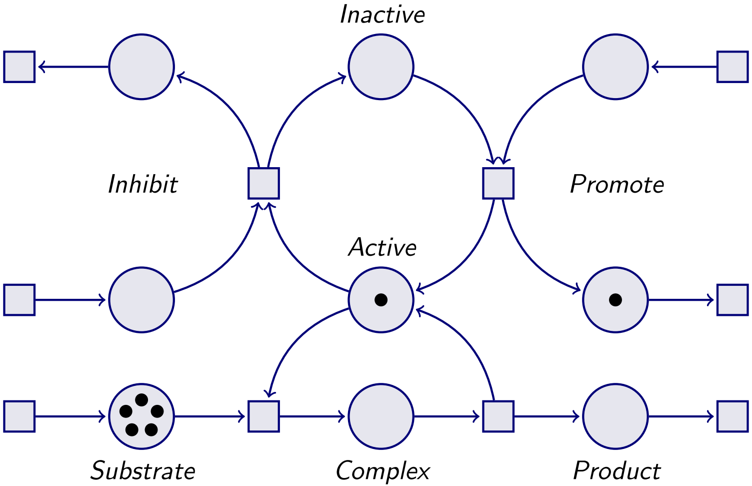

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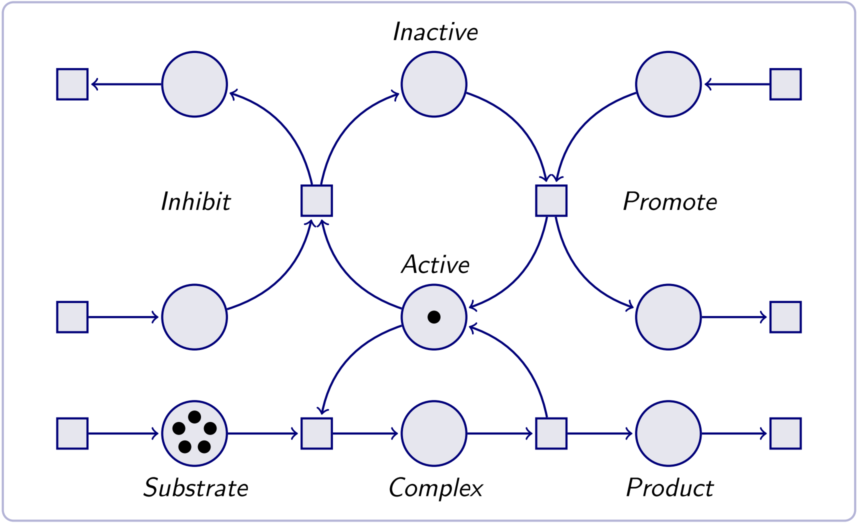


Other activities

Appropriate Petri nets can model a wide range of activities:

- Creation, transport, degradation
- Chemical reactions $A + A + B \rightarrow AB$
- Reversible reactions $P + Q \leftrightharpoons PQ$
- Promotion, inhibition
- Cascades, signal transduction
- Feedback, feedforward
- ...

These can then be chained together into larger nets to model more substantial systems. As in, for example, the Petri Net Pathways database:

http://genome.ib.sci.yamaguchi-u.ac.jp/~pnp/

Note that all these are *discrete* state space, *nondeterministic*, *untimed* and generally *qualitative* models of the system of interest.

Outline

Formal presentation of nets

We can describe any Petri Net as a tuple:

$$(P, T, Pre, Post)$$

where

$$\begin{array}{ll} P & \text{is a finite set of places} \\ T & \text{is a finite set of transitions, disjoint from } P \end{array}$$

$$\begin{array}{rl} Pre : T \times P \to \mathbb{N} & \text{Pre-state weighting} \\ Post : T \times P \to \mathbb{N} & \text{Post-state weighting} \end{array}$$

From these we obtain two derived notions:

$$\begin{array}{rl} M : P \to \mathbb{N} & \text{Marking of places with tokens} \\ X : T \to \mathbb{N} & \text{Multiset of simultaneous transitions} \end{array}$$

Net dynamics

The dynamics of a net (P,T, Pre, Post) are given by a relation between markings and transitions:

$$M \xrightarrow{X} N \overset{def}{\iff}$$
$$\forall p \in P\,.\, M(p) \geqslant \sum_{t \in T} X(t)Pre(t,p)$$
$$\&\ \forall p \in P\,.\, N(p) = M(p) - \sum_{t \in T} X(t)Pre(t,p) + \sum_{t \in T} x(t)Post(t,p)$$

Individual transitions are a special case of this, where the multiset X has just one element.

A transition X is *enabled* in marking M if the first of these conditions holds $\forall p \in P\,.\, M(p) \geqslant \sum_{t \in T} X(t)Pre(t,p)$.

Given an initial marking M_0, a marking N is *reachable* if there is some sequence of transitions

$$M_0 \xrightarrow{X_0} M_1 \xrightarrow{X_1} M_2 \ldots M_k \xrightarrow{X_k} N$$

Outline

1. Example Petri Nets
2. Formalities
3. Matrix representation
4. Closing

Matrix presentation

The components of a Petri net can be conveniently represented as matrices.

Given finite sets P of places and T of transitions, then

- Pre-state weighting Pre is a $T \times P$ matrix of natural numbers
- Post-state weighting Post is a $T \times P$ matrix of natural numbers

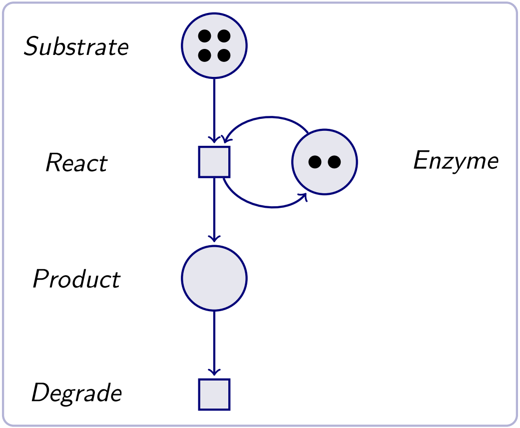
- A marking M is a P-element vector of natural numbers
- A transition X is a T-element vector of natural numbers

Transition X is enabled in marking M if $M \geqslant \mathrm{Pre}\, X$

$$
\begin{aligned}
M \xrightarrow{X} N \iff M \geqslant \mathrm{Pre}\, X \;\&\; N &= M - \mathrm{Pre}\, X + \mathrm{Post}\, X \\
&= M + AX \quad \text{where } A = (\mathrm{Post} - \mathrm{Pre})
\end{aligned}
$$

The matrix A (or its transpose) is variously known as the *incidence*, *reaction* or *stoichiometry* matrix of the net.

Matrix Example



$$\text{Pre} = \begin{array}{c} R \quad T \\ \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \end{array} \begin{array}{l} \textit{Substrate} \\ \textit{Enzyme} \\ \textit{Product} \end{array}$$

$$\text{Post} = \begin{array}{c} R \quad T \\ \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \end{pmatrix} \end{array} \begin{array}{l} \textit{Substrate} \\ \textit{Enzyme} \\ \textit{Product} \end{array}$$

$$\text{M} = \begin{pmatrix} 4 \\ 2 \\ 0 \end{pmatrix} \begin{array}{l} \textit{Substrate} \\ \textit{Enzyme} \\ \textit{Product} \end{array}$$

Outline

Homework

Build small Petri nets to illustrate some of these activities:

- Creation, transport, degradation
- Chemical reactions $A + A + B \rightarrow AB$
- Reversible reactions $P + Q \leftrightharpoons PQ$
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Draw them and record their details in matrix form.