Math 2300 **DISCRETE MATH** Spring 2010
Dr. Duval **Project 3**
due Wendesday, May 5

Reaction Networks and Petri Nets

In this project, we'll use graphs to analyze reaction networks. In particular, we'll model these with Petri nets, an abstraction also used in more general computational settings beyond reaction networks.

The building blocks of reaction networks are chemical reactions, which, for our purposes, will be the production of some "products" (outputs) from some "reactants" (inputs). A reaction network is a series of chemical reactions with the products of some reactions being the reactants of others. In practice, this overlap of reactants and products should be large enough, and interrelated enough, to warrant drawing a diagram, though it's not strictly necessary.

An example of a reaction network is the following auto-regulation network from *Stochastic Modelling for Systems Biology*, by Darren J. Wilkinson:

$$\begin{aligned}
g + P2 &\to gP2 \\
gP2 &\to g + P2 \\
g &\to g + r \\
r &\to r + P \\
2P &\to P2 \\
P2 &\to 2P \\
r &\to \emptyset \\
P &\to \emptyset
\end{aligned}$$

[Notes: $2P$ means $P + P$ but the "2" in $P2$ and $gP2$ has no significance for us; $\emptyset$ on the right side of an arrow means there is no product from that reaction, i.e., the reaction simply consumes the reactant.]

A Petri net is one way of illustrating this network. It starts with a Petri net graph, a specific kind of directed graph. Every substance (reactant and/or product) in any of the reactions gets a vertex, typically depicted with a circle, and called a "place" (for clarity, I'll say "place vertex"); and every reaction also get a vertex, typically depicted with a rectangle or a thick line, and called a "transition" (for clarity, I'll say "transition vertex"). The directed edges are drawn as follows: For each reaction, directed edges go from (the vertices of) the reactants of that reaction towards (the vertex of) the reaction, and also go from (the vertex of) the reaction towards the (the vertices of) the products of the reaction. (The reactants will all point towards one long side of the rectangle representing a reaction, while its products will all point out of the opposite long side of the rectangle.) See the example in Figure 1; the "2" on some edges is shorthand for a pair of directed edges pointing that way, and corresponds to the "2" in "$2P$" in the appropriate reaction.

To now make a Petri net out of the Petri net graph, we need to put some quantities of each substance into the graph, and simulate the reactions. To do this, we further specify

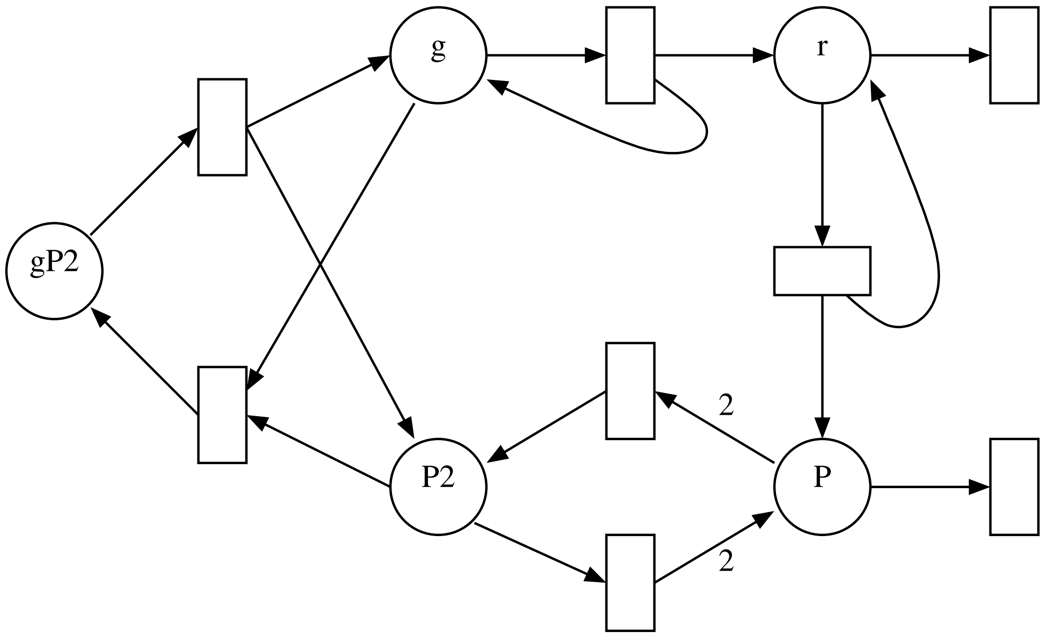

Figure 1: Petri net graph

that each place vertex is assigned a number of "tokens", which represent quantities of the associated substance. The number of tokens must be a non-negative integer. (The number is non-negative because you can't have a negative quantity of a substance; it is an integer largely for convenience, though one can think of this number as counting molecules.) Once the initial number of tokens has been placed on the vertices, we "fire" a transition vertex if there is at least one token on each of its reactants; in this case, each reactant vertex of the reaction loses one token (to the reaction) and each product vertex of the same reaction gains one token (from the reaction). Note that there may be more than one transition vertex ready to fire, but we only fire one transition vertex one at a time. There is no tiebreaking rule to determine which of these several vertices will fire first (which makes this a "nondetetrministic" system).

For instance, we could put tokens on the place vertices as shown in Figure 2. Because there are no tokens on the $gP2$ vertex, we cannot fire the transition vertex corresponding to the $gP2 \to g + P2$ reaction, though we can fire the other transition vertices. After firing the transition vertices corresponding to the reactions $g + P2 \to gP2$ and $r \to r + P$ the tokens are now arranged as shown in Figure 3.

1. Explain why Petri net graphs are always bipartite.

2. What does the indegree and outdegree of each place vertex in a Petri net graph mean? What does the indegree and outdegree of each transition vertex in a Petri net graph mean?

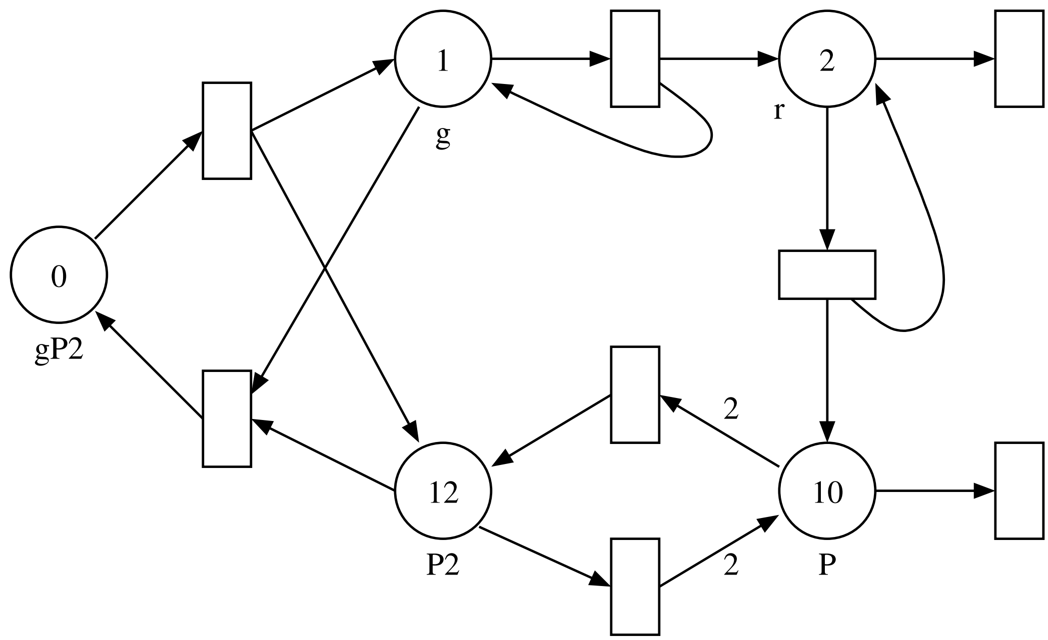

Figure 2: Petri net with tokens

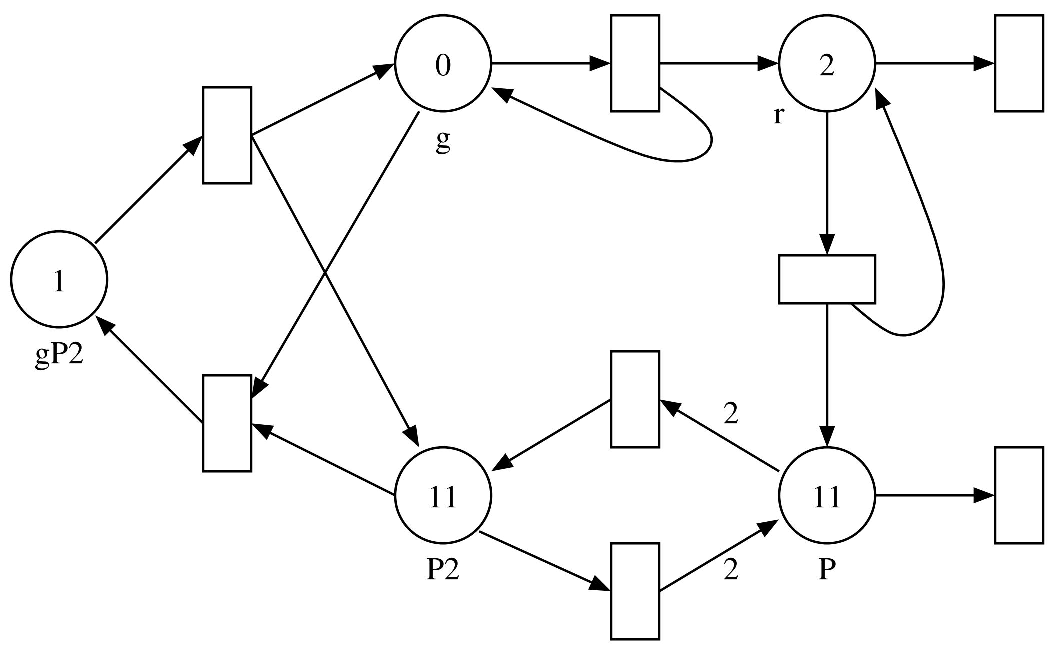

Figure 3: Petri net after reactions

3. Draw the Petri net graph for the following reaction network for (a very simplified model of) sexual reproduction (an example from population biology, instead of biochemistry):

$$\begin{aligned} M + F &\to L \\ L &\to 2m + 2f \\ R + m &\to M \\ R + f &\to F \end{aligned}$$

[M stands for adult males, F stands for adult females, m stands for male children, f stands for female children, L stands for litters and R stands for resource.]

4. Make the Petri net graph you just drew into a Petri net by initially assigning tokens to the place vertices as follows:

place	tokens
M	10
F	10
m	0
f	0
L	0
R	100

Show what happens to the Petri net as you fire transition vertices. Perform a sequence of at least six firings.

5. There are many interesting things we can do with Petri nets. One is to look at "reachability", the question of whether a given arrangement of tokens can be reached from another arrangement through a series of firings. To solve this problem in general is hard. To get a feel for it, show that the following arrangement of tokens in the above Petri net is reachable from the initial arrangement given above.

place	tokens
M	15
F	25
m	10
f	0
L	0
R	50

Describe what you did to figure out that this arrangement is reachable. [It is not sufficient to say something like "I tried a bunch of things, and this worked." Really explain in some detail what you did.]

6. Make your own Petri net with a starting assignment of tokens, and find an arrangement that is **not** reachable from this starting assignment. Explain **why** this arrangement is not reachable. [Hint: It does not have to be large.]