Problem Set 2

- You may use your course materials and/or any literature resources (as well as the internet) to formulate your solution.
- Your solution must be submitted as a Pluto notebook starting from the template notebook on GitHub. The link to the repository holding the final solution notebook should be submitted to the teaching team email.
- You may work in teams. Each student on a team must be a collaborator on the GitHub repository, and the roles/responsibilities of each team member must be described in the notebook.
- All lecture routines required for this problem set are available in the template notebook and pre-loaded upon notebook startup.
- Problem Set 2 is due on **T, Feb 18, 2022** by **4:59 PM**.

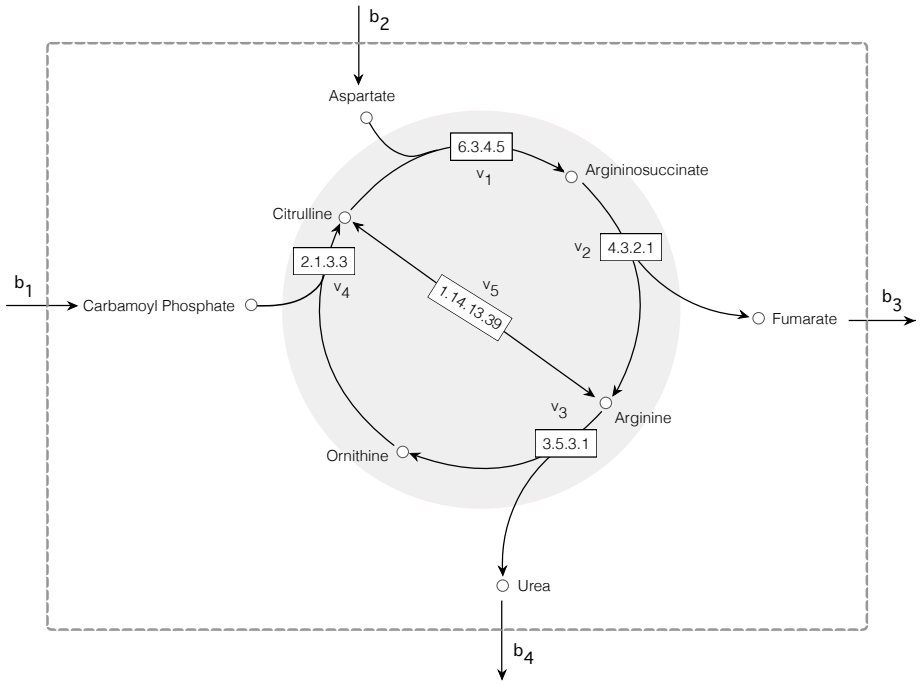

Figure 1: Schematic of the Urea cycle.

1. The urea cycle eliminates excess nitrogen from the cell (Fig. 1). Let's analyze the structure of this reaction network by formulating the stoichiometric matrix $\mathbf{S}$, and computing the reaction/metabolite extreme pathways and connectivity arrays.

    a) Use KEGG (Arginine biosynthesis in human) to construct the stoichiometric matrix **S** for the urea cycle shown in Fig. 1. The KEGG link is: `https://www.genome.jp/kegg-bin/show_pathway?hsa00220`. **Note**: additional exchange reactions $b_\star$ may be required beyond those shown in Fig. 1.

    b) Compute the extreme pathway array $\mathbf{P}$ for your urea cycle reconstruction using the `expa` routine.

        – How many extreme pathways (rows of $\mathbf{P}$) did you get, and how many produced Urea?

        – Compute the reaction frequency (fraction of extreme pathways using a particular reaction) for each reaction (cols of $\mathbf{P}$).

    c) Compute the metabolite and the reaction connectivity arrays. Rank order (from most to least) the connectivity of the metabolites and reactions.

        – Is there a correlation between reaction connectivity and extreme pathway reaction frequency?